III MODEL CALCULATIONS

In this chapter, the model equations are presented with a short explanation of the modelled processes. For background and discussion on these model approaches, the reader is referred to Chapter II and the TGD (EC, 2003). Chapter III follows the same structure as the previous chapter; the modules and sub-modules described in Chapter II are handled separately.

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III.1 INTRODUCTION

This chapter, the model calculations of the system are specified in detail. As discussed in the previous chapter, the system consists of six main modules: Input, Release Estimation, Environmental Distribution, Exposure Assessment, Effects Assessment and Risk Characterisation. In several modules, sub-modules are distinguished when the calculations describe a specific, well-defined process. As an example, the environmental distribution module has a separate sub-module describing sewage treatment. Each module or sub-module is first described by the parameters that are required for the calculations (input), the intermediate results (which are also shown to the user), and the resulting parameters used in subsequent calculations (output). The parameters are presented in the following manner:

Input

[Symbol]	[Description of required parameter]	[Unit]	

These parameters are the input to the module. They may be derived either from the data set, or from the output of other modules.

Intermediate results

[Symbol]	[Description of intermediate parameter]	[Unit]	^{c}

These parameters are the results of the calculations in this module, but are not used in other modules. They are output to the screen to give the user the opportunity to modify these results. In some modules, several levels of intermediate results are specified when an intermediate parameter influences another intermediate parameter.

Output

[Symbol]	[Description of resulting parameter]	[Unit]	^{c}

These parameters are the results of the calculations in this module which are used in other modules. In some modules, several levels of output are specified when an output parameter influences another output parameter.

For the explanation of symbols used in an equation, the same table format is used:

Input			
[Symbol]	[Description of required parameter]	[Unit]	S/D/O/P/^{c}/*
Output			
[Symbol]	[Description of resulting parameter]	[Unit]	O/^{c}/*

The S, D, O or P classification of a parameter indicates the status:

S	Parameter must be present in the input data set for the calculation to be executed (there is no method implemented in the system to estimate this parameter; no default value is set).
D	Parameter has a standard default value (most defaults can be changed by the user). Defaults are presented in the sub-module, where they are used in separate tables. Sets of changed default values can be saved.
U	This parameter is 'unspecified', no default value is set.
O	Parameter is output from another calculation (most output parameters can be overwritten by the user with alternative data).
P	Parameter value can be chosen from a 'pick-list' with values.
^{c}	Default or output parameter is closed and cannot be changed by the user.
*	An asterisk is added when a parameter can be set to a different value on the regional and continental spatial scale.

For the symbols, as far as possible, the following conventions are applied:

- Parameters are mainly denoted in capitals.
- Specification of the *parameter* is in lower case.
- Specification of the *compartment* for which the parameter is specified is shown as a subscript.

The following symbols are frequently used:

E	for emissions (direct and indirect via STP)	[kg.d^{-1}]
F	for 'dimensionless' fractions	[kg.kg^{-1}] or [m^3.m^{-3}]
C	for the concentration of a chemical	[kg$_c$.kg^{-1}] or [kg$_c$.m^{-3}]
RHO	for densities of compartments or phases	[kg.m^{-3}]
K	for inter-media partition coefficients	[-] or [m^3.kg^{-1}]
k	for rate constants (e.g. degradation rates)	[d^{-1}]
DT50	for half-lives	[d]
T	for a fixed period of time (e.g. an exposure period)	[d]
TEMP	for temperature	[K]
DEPTH	for soil or water depth	[m]
PEC	for Predicted Environmental Concentrations	[kg$_c$.kg^{-1}] or [kg$_c$.m^{-3}]
PNEC	for Predicted No-Effect Concentrations	[kg$_c$.kg^{-1}] or [kg$_c$.m^{-3}]
RCR	for Risk Characterisation Ratios	[-]

As an example, the symbol Foc_{soil} means the fraction (*F*) organic carbon (*oc*) in the soil compartment ($_{soil}$). For other parameters, interpretable symbols are chosen. SI units are applied for the sake of consistency in the program. As a consequence, some parameters have an uncommon unit (e.g. *Kp* will internally have the unit m^3.kg^{-1} instead of the more commonly used l.kg^{-1}). Kilograms of chemical are indicated by the unit kg$_c$. Other kilograms will usually be indicated as wet weight or dry weight (kg$_{wwt}$ and kg$_{dwt}$, respectively). It should be noted that for the dimension 'time' the non-SI unit 'days' is used, since this is a more relevant unit in the framework of risk assessment.

The equations in this chapter are numbered. The same equation numbering is also used in the EUSES on-line help and in the code of the program.

III.2 INPUT MODULE

In the input module, the basic scope of the assessment is selected and basic substance information must be entered. This includes substance identification and physico-chemical properties. Other input data such as toxicity data or measured partition coefficients can be entered in the dedicated sub-modules.

III.2.1 Assessment types

The user of EUSES is able to determine the scope of the risk assessment at the start of the program. It is possible to choose between:

Assessment types

Environmental assessment of Biocides (biocides, non-agricultural) on the <u>local scale only</u>

I Environmental assessment (local scale).
II Assessment for predators exposed via the environment (local scale).
III Assessment for humans exposed via the environment (local scale).
IV Assessment for humans exposed to or via consumer products (non-professional user).

New and Existing Substances and Biocides

I Environmental assessment, with two options:
  Ia local scale
  Ib regional scale
II Assessment for predators exposed via the environment (both scales combined)
III Assessment for humans exposed via the environment, with two options:
  IIIa local scale
  IIIb regional scale
IV Assessment for humans exposed to or via consumer products.
V Assessment for humans exposed at the workplace.

Hydrocarbon Block method

- Block method for mixtures, local and regional scale

The calculations for the different assessment types are given in Sections III.3 to III.7. The specific differences in the assessment with the Hydrocarbon Block Method and the additional requirements for assessment of metals and metal compounds are described in Section III.8 and III.9.

III.2.2 Input data

The following data on substance identification and physicochemical data need be entered in this module.

Also data on partition coefficients and bioconcentration factors, on degradation and transformation and on removal rates constants for soil can be entered in this module. Information on these data can be found in the chapter 4.1 (partition coefficients), 4.2 (degradation and transformation rates), 4.4.6 (bioconcentration factor for aquatic biota) 4.5.4 (removal rate constants local soil), 5.1 and 5.2 (bioconcentration factors for secondary poisoning and human exposure). The input data can be related to the Kow (using a QSAR or Koc), have defaults that can be overwritten or are calculated from other parameters and can be overwritten. Besides, information on biodegradation is needed.

Substance identification input		
	general name	
	CAS no.	
	EC notification no.	
	EINECS no.	
Physico-chemical properties input		
MOLW	molecular weight	$[kg_c.mol^{-1}]$
Kow	octanol-water partition coefficient	[-]
$VPtemp_{test}$	vapour pressure at the temperature of the data set	[Pa]
$SOLtemp_{test}$	water solubility at the temperature of the data set	$[kg_c.m^{-3}]$
TEMPtest	temperature of the measured physico-chemical data	[K]
TEMPboil	boiling point (used for some release estimations and EASE)	[K]
TEMPmelt	melting point (used for solids only and for EASE)	[K]
Physico-chemical properties output		
$VPtemp_{env}$	vapour pressure at the environmental temperature	[Pa]
$SOLtemp_{env}$	water solubility at the environmental temperature	$[kg_c.m^{-3}]$

Table III-1 *Defaults for the physico-chemical properties input*

Parameter	**Symbol**	**Unit**	**Value**
Enthalpy of vaporisation	H_{0_VP}	$[J.mol^{-1}]$	5.10^4
Enthalpy of solution	H_{0_SOL}	$[J.mol^{-1}]$	1.10^4
Gas constant	R	$[Pa.m^3.mol^{-1}.K^{-1}]$	8.314 [a]
Environmental temperature	TEMP	[K]	
Freshwater environment (12 °C)			285
Marine environment (12 °C)			285[b]

[a] This default cannot be changed by the user.

[b] Although the TGD (2003) proposed a temperature of 9 °C, due to the small differences it was decided to keep the temperature the same for all compartments on the moderate global scale the same.

Experimentally derived chemical properties will usually be measured at a standard temperature, which is different from the temperature used in the models of EUSES. For most chemicals and most properties, a temperature correction will not be necessary between the standard 20 or 25 degrees and the environmental temperature used in the system (by default 12 °C in the environment and 15 °C in the STP). When experimentally determined physico-chemical data have been obtained at a temperature which, for the substance under consideration, would significantly change when extrapolated to the relevant temperature of the exposure models employed, then a temperature correction should be considered.

The vapour pressure may for some substances change considerably according to the temperature even within a temperature range of only 10 °C. In this case a general temperature correction should be applied according to the following equation:

$$VPtemp_{env} = VPtemp_{test} \cdot e^{\left(\frac{H_{0\_VP}}{R} \cdot \left(\frac{1}{TEMPtest} - \frac{1}{TEMPenv}\right)\right)} \qquad \textbf{(1)}$$

Care must be taken when the melting point is within the extrapolated temperature range. The vapour pressure of the solid phase is always lower than the extrapolated vapour pressure of the liquid phase.

The same approach can be followed for correcting the water solubility:

$$SOLtemp_{env} = SOLtemp_{test} \cdot e^{\left(\frac{H_{0\_SOL}}{R} \cdot \left(\frac{1}{TEMPtest} - \frac{1}{TEMPenv}\right)\right)} \qquad \textbf{(2)}$$

Input			
$VPtemp_{test}$	vapour pressure at the temperature of the data set	[Pa]	S
$SOLtemp_{test}$	water solubility at the temperature of the data set	$[kg_c.m^{-3}]$	S
H_{0_VP}	enthalpie of vapourisation	$[J.mol^{-1}]$	D
H_{0_SOL}	enthalpie of solution	$[J.mol^{-1}]$	D
R	gas constant	$[Pa.m^3.mol^{-1}.K^{-1}]$	D
TEMPtest	temperature of the measured physico-chemical data	[K]	S
TEMPenv	environmental temperature	[K]	D
Output			
$VPtemp_{env}$	vapour pressure at the environmental temperature	[Pa]	O
$SOLtemp_{env}$	water solubility at the environmental temperature	$[kg_c.m^{-3}]$	O

III.3 RELEASE ESTIMATION FOR NEW AND EXISTING SUBSTANCES AND BIOCIDES

Releases to all spatial scales are estimated, based on use pattern and substance properties. The tables in Appendix III provide default release estimates for each category of substance. Release estimation applies either the tonnage of the substance as a starting point or representative dimensions (quantities, concentrations, etc.) for the process or the average consumption. In both cases emission factors (fractions released to the relevant environmental compartments) are used. These emission factors have been collected in the A-tables of Appendix III. In the TGD the A-tables the (realistic) worst case estimates are based on expert judgement and in some cases on use category documents. In this version of EUSES the emission factors of specific emission scenario documents of the TGD have been incorporated.

The B-tables of the TGD contain data to determine the estimates for the daily quantity applicable for each relevant stage of the life cycle based on the tonnage. In this version of EUSES specific data on representative source size of the emission scenario documents of the TGD have been incorporated as well.

It should be noted that release estimation using average capacities or consumption concerns the local scale only. For the regional scale an "overall" emission factor should be used.

Input: use pattern of the substance			
PRODVOL	production volume of chemical in EU	[kg$_c$.d^{-1}]	
HPVC	high-production volume chemical	[yes/no]	
IMPORT	volume of chemical imported to EU	[kg$_c$.d^{-1}]	
EXPORT	volume of chemical exported from EU	[kg$_c$.d^{-1}]	
INDCAT	industrial category	[-]	
USECAT	use category	[-]	
MAINCAT	main category (for existing substances)	[-]	
Ftonnage$_k$	fraction of tonnage for application *k*	[-]	
Fchem$_{form}$	fraction of chemical in formulation	[-]	
	relevant steps in life cycle		
	specific information on substance use pattern		
Input: physico-chemical properties			
SOL	water solubility	[kg$_c$.m^{-3}]	
VP	vapour pressure	[Pa]	
MOLW	molecular weight	[kg$_c$.mol^{-1}]	
TEMPboil	boiling point (for some release estimations only)	[K]	
Intermediate results 1			
TONNAGE	tonnage in EU	[kg$_c$.d^{-1}]	
TONNAGE$_k$	relevant tonnage for application *k* in EU	[kg$_c$.d^{-1}]	
PRODVOLreg	production volume of chemical in region	[kg$_c$.d^{-1}]	
TONNAGEreg	tonnage in region	[kg$_c$.d^{-1}]	
TONNAGEreg$_{form}$	regional tonnage of formulation used	[kg$_c$.d^{-1}]	c
PRODVOLcont	production volume of chemical in continent	[kg$_c$.d^{-1}]	c
TONNAGEcont	tonnage in continent	[kg$_c$.d^{-1}]	c
Intermediate results 2			
F$_{i,j}$	fraction of tonnage released during stage *i* to compartment *j*	[-]	
Fmainsource$_i$	fraction of the main local source during life-cycle stage *i*	[-]	
Temission$_i$	number of days per year for the emission in stage *i*	[d.yr^{-1}]	
Intermediate results 3			
RELEASEreg$_{i,j}$	regional release during life-cycle stage *i* to compartment *j*	[kg$_c$.d^{-1}]	
RELEASEcont$_{i,j}$	continental release during life-cycle stage *i* to compartment *j*	[kg$_c$.d^{-1}]	
Output			
Elocal$_{i,j}$	local emission during episode to comp. *j* during stage *i*	[kg$_c$.d^{-1}]	
Temission$_i$	number of days per year for the emission in stage *i*	[d.yr^{-1}]	
Ereg$_j$	total regional emission to compartment *j* (annual average)	[kg$_c$.d^{-1}]	
Ereg$_{direct\text{-}water}$	direct regional emission to surface water (annual average)	[kg$_c$.d^{-1}]	
Econt$_j$	total continental emission to compartment *j* (annual average)	[kg$_c$.d^{-1}]	
Econt$_{direct\text{-}water}$	direct continental emission to surface water (annual average)	[kg$_c$.d^{-1}]	

With:

i	stage of the life cycle	*j*	compartment
1	production	air	air
2	formulation	water	(waste) water
3	industrial use	ind	industrial soil (regional scale only)
4	private use	surf	surface water (regional scale only)
5	service life	agric	agricultural soil (regional only, no estimation
6	waste treatment		

Table III-2 Defaults for emission calculations.

Parameter	Symbol	Unit	Value
Fraction of EU production volume of substance produced in the region	$Fprodvol_{reg}$	[-]	1 [a]
Fraction connected to sewer systems	$Fconnect_{stp}$	[-]	0.80

a For life cycle stage Private use the default remains 0.10.

III.3.1 Calculation of the tonnage of substance

The total production volume in the EU is available in the data set and denoted by *PRODVOL*. *TONNAGE* is the volume of substance that is used for subsequent life-cycle stages.

$$TONNAGE = PRODVOL + IMPORT - EXPORT \qquad (3)$$

Input

PRODVOL	production volume of chemical in EU	$[kg_c.d^{-1}]$	S
IMPORT	volume of chemical imported to EU	$[kg_c.d^{-1}]$	S
EXPORT	volume of chemical exported from EU	$[kg_c.d^{-1}]$	S

Output

TONNAGE	tonnage of substance in EU	$[kg_c.d^{-1}]$	O

When a substance has more than one application, the tonnage must be broken down for the different, relevant applications (indicated by the index *k*). Each application has a different combination of industrial and use category (INDCAT/USECAT).

$$TONNAGE_k = Ftonnage_k \cdot TONNAGE \qquad (4)$$

Input

TONNAGE	total tonnage of substance in EU	$[kg_c.d^{-1}]$	O
$Ftonnage_k$	fraction of total tonnage for application *k*	[-]	S

Output

$TONNAGE_k$	relevant tonnage for application *k* in EU	$[kg_c.d^{-1}]$	O

This also implies that all parameters depending on the tonnage should also receive a subscript *k* (e.g. releases, environmental concentrations, risk characterisation ratios). This is not shown in this rest of this documentation.

It should be noted that the production volume is *not* broken up according to this fraction since a chemical is usually produced according to one production method (independent of subsequent usages). In the program, production *can* be set to 'relevant' for more than one usage. In that case, each production stage can be calculated with the relevant percentage of the total production volume.

If application *k* concerns a biocide the life cycle stages concerning the application – such as industrial use – have to be evaluated separately (see section III.2.1. Assessment types). This can only be done for the local scale. The calculations are presented in III.3.6.

A fixed fraction of total EU production and tonnage is assumed for the standard region. The regional and continental fate calculations are done with a nested multimedia model (as explained in Section II.4.4). Therefore, the produced volume and tonnage for the continental box must exclude the values for the regional system.

$$\boldsymbol{PRODVOLreg = Fprodvol_{reg} \cdot PRODVOL} \qquad \textbf{(5)}$$

$$\boldsymbol{PRODVOLcont = (1 - Fprodvol_{reg}) \cdot PRODVOL} \qquad \textbf{(6)}$$

$$\boldsymbol{TONNAGEreg = Fprodvol_{reg} \cdot TONNAGE} \qquad \textbf{(7)}$$

$$\boldsymbol{TONNAGEcont = (1 - Fprodvol_{reg}) \cdot TONNAGE} \qquad \textbf{(8)}$$

Input			
PRODVOL	production volume of chemical in EU	[$kg_c.d^{-1}$]	S
TONNAGE	tonnage of substance in EU	[$kg_c.d^{-1}$]	O
$Fprodvol_{reg}$	fraction of production volume for region	[-]	D
Output			
PRODVOLreg	regional production volume of substance	[$kg_c.d^{-1}$]	O
TONNAGEreg	regional tonnage of substance	[$kg_c.d^{-1}$]	O
PRODVOLcont	continental production volume of substance	[$kg_c.d^{-1}$]	O^c
TONNAGEcont	continental tonnage of substance	[$kg_c.d^{-1}$]	O^c

III.3.2 Releases during each life-cycle stage

III.3.2.1 Release information from A and B-tables of Appendix III

The fractions released at every relevant stage of the life cycle and to every relevant compartment are derived from the A-tables in Appendix III. These fractions are denoted by $F_{i,j}$, where *i* is the stage in the life cycle and *j* is the compartment. For the local assessments, the B-tables provide the fraction from a main point source and the expected number of emission days per year. In the A and B-tables of Appendix III, the production volume for the region (*PRODVOLreg*) must be used for *T* at the stage of production. *TONNAGEreg* should be used for the subsequent life-cycle stages. It should be noted that in the emission tables, the production volume or tonnage is expressed in tonnes/year. When a chemical is applied in a formulation at a rather low level, the tonnage must be corrected to the tonnage of the total formulation. This tonnage is only used to retrieve the correct fraction of the main source and number of emission days from the B-tables.

$$TONNAGEreg_{form} = \frac{1}{Fchem_{form}} \cdot TONNAGEreg \qquad \textbf{(9)}$$

Input			
TONNAGEreg	regional tonnage of substance	$[kg_c.d^{-1}]$	O
$Fchem_{form}$	fraction of chemical in formulation	[-]	S
Output			
$TONNAGEreg_{form}$	regional tonnage of formulation used	$[kg_c.d^{-1}]$	O^c

Input for A and B tables in Appendix III			
PRODVOLreg	regional production volume of chemical (stage of production)	$[kg_c.d^{-1}]$	O
TONNAGEreg	regional tonnage of substance (A-tables)	$[kg_c.d^{-1}]$	O
$TONNAGEreg_{form}$	regional tonnage of substance (B-tables)	$[kg_c.d^{-1}]$	O^c
HPVC	high-production volume chemical	[yes/no]	P
INDCAT	industrial category	[-]	P
USECAT	use category	[-]	P
MAINCAT	main category (for existing substances)	[-]	P
SOL	water solubility	$[kg_c.m^{-3}]$	S
VP	vapour pressure	[Pa]	S
MOLW	molecular weight (only used to estimate log Henry in Table A3.7 for industrial use in IC=8)	$[kg_c.mol^{-1}]$	S
TEMPboil	boiling point (only for some release estimations)	[K]	S
Output from A tables in Appendix III			
$F_{i,j}$	fraction of tonnage released during stage *i* to compartment *j*	[-]	O
Output from B tables in Appendix III			
$Fmainsource_i$	fraction of the main local source during life cycle stage *i*	[-]	O
$Temission_i$	number of days per year for the emission in stage *i*	$[d.yr^{-1}]$	O

In case there is more than one usage of a chemical, the emission tables are accessed with the regional tonnage $TONNAGEreg_k$ derived from Equation (4) and (7). It should be noted that the production volume is *not* broken up. In case the Block Method is used (see Section III.8) the total tonnage/production volume is used to access the tables. The break up for the separate blocks is done in the calculation of the releases to each compartment (Sections III.3.2.2 and III.3.2.3).

III.3.2.2 Continental releases

The annual average release per stage of the life cycle can be calculated with the following series of equations. For each relevant stage, the losses in the previous stage are taken into account. Note that releases during production are *not* taken into account in the other stages, as these releases will generally already be accounted for in the reported production volume.

1. production
$RELEASEcont_{1,j}$:
air $F_{1,\,air} \cdot PRODVOLcont$
water $F1,\ water \cdot PRODVOLcont$
soil $F_{1,\,ind} \cdot PRODVOLcont$
surf $F_{1,\,surf} \cdot PRODVOLcont$
total $\Sigma F_{1,j} \cdot PRODVOLcont$
amount used: $TONNAGEcont$

2. formulation
$RELEASEcont_{2,j}$:
air $F_{2,\,air} \cdot TONNAGEcont$
water $F_{2,\,water} \cdot TONNAGEcont$
soil $F_{2,\,ind} \cdot TONNAGEcont$
surf $F_{2,\,surf} \cdot TONNAGEcont$
total $\Sigma F_{2,j} \cdot TONNAGEcont$
rest: $(1-\Sigma F_{2,j}) \cdot TONNAGEcont$

3. industrial use
$RELEASEcont_{3,j}$:
air $F_{3,\,air} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEcont$
water $F_{3,\,water} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEcont$
soil $F_{3,\,ind} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEcont$
surf $F_{3,\,surf} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEcont$
total $\Sigma F_{3,j} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEcont$

4. private use
$RELEASEcont_{4,j}$:
air $F_{4,\,air} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEcont$
water $F_{4,\,water} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEcont$
soil $F_{4,\,ind} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEcont$
surf $F_{4,\,surf} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEcont$
total $\Sigma F_{4,j} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEcont$
rest: $(1-\Sigma F_{3,j} - \Sigma F_{4,j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEcont$

5. service life
$RELEASEcont_{5,j}$:
air $F_{5,\,air} \cdot (1-\Sigma F_{3,j} - \Sigma F_{4,j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEcont$
water $F_{5,\,water} \cdot (1-\Sigma F_{3,j} - \Sigma F_{4,j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEcont$
soil $F_{5,\,ind} \cdot (1-\Sigma F_{3,j} - \Sigma F_{4,j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEcont$
surf $F_{5,\,surf} \cdot (1-\Sigma F_{3,j} - \Sigma F_{4,j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEcont$
total $\Sigma F_{5,j} \cdot (1-\Sigma F_{3,j} - \Sigma F_{4,j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEcont$

6. waste treatment

$RELEASEcont_{5,j}$:

air	$F_{6,\,air} \cdot (1\text{-}\Sigma F_{3,\,j} - \Sigma F_{4,\,j} - \Sigma F_{5,\,j}) \cdot (1\text{-}\Sigma F_{2,j}) \cdot TONNAGEcont$
water	$F_{6,\,water} \cdot (1\text{-}\Sigma F_{3,\,j} - \Sigma F_{4,\,j} - \Sigma F_{5,\,j}) \cdot (1\text{-}\Sigma F_{2,j}) \cdot TONNAGEcont$
soil	$F_{6,\,ind} \cdot (1\text{-}\Sigma F_{3,\,j} - \Sigma F_{4,\,j} - \Sigma F_{5,\,j}) \cdot (1\text{-}\Sigma F_{2,j}) \cdot TONNAGEcont$
surf	$F_{6,\,surf} \cdot (1\text{-}\Sigma F_{3,\,j} - \Sigma F_{4,\,j} - \Sigma F_{5,\,j}) \cdot (1\text{-}\Sigma F_{2,j}) \cdot TONNAGEcont$
total	$\Sigma F_{6,\,j} \cdot (1\text{-}\Sigma F_{3,\,j} - \Sigma F_{4,\,j} - \Sigma F_{5,\,j}) \cdot (1\text{-}\Sigma F_{2,j}) \cdot TONNAGEcont$

Input			
$F_{i,j}$	fraction of tonnage released during stage *i* to compartment *j*	[-]	O
PRODVOLcont	production volume of substance in continent	$[kg_c.d^{-1}]$	O
TONNAGEcont	tonnage of substance in continent	$[kg_c.d^{-1}]$	O
Output			
$RELEASEcont_{i,j}$	continental release during life-cycle stage *i* to compartment *j*	$[kg_c.d^{-1}]$	O

III.3.2.3 Regional releases

1. production

$RELEASEreg_{1,j}$:
air $F_{1,air} \cdot PRODVOLreg$
water $F_{1,water} \cdot PRODVOLreg$
soil $F_{1,ind} \cdot PRODVOLreg$
surf $F_{1,surf} \cdot PRODVOLreg$
total $\Sigma F_{1,j} \cdot PRODVOLreg$
amount used: $TONNAGEreg$

2. formulation

$RELEASEreg_{2,j}$:
air $F_{2,air} \cdot TONNAGEreg$
water $F_{2,water} \cdot TONNAGEreg$
soil $F_{2,ind} \cdot TONNAGEreg$
surf $F_{2,surf} \cdot TONNAGEreg$
total $\Sigma F_{2,j} \cdot TONNAGEreg$
rest: $(1-\Sigma F_{2,j}) \cdot TONNAGEreg$

3. industrial use

$RELEASEreg_{3,j}$:
air $F_{3,air} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEreg$
water $F_{3,water} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEreg$
soil $F_{3,ind} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEreg$
surf $F_{3,surf} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEreg$
total $\Sigma F_{3,j} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEreg$

4. private use

$RELEASEreg_{4,j}$:
air $F_{4,air} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEreg$
water $F_{4,water} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEreg$
soil $F_{4,ind} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEreg$
surf $F_{4,surf} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEreg$
total $\Sigma F_{4,j} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEreg$
rest: $(1-\Sigma F_{3,j} - \Sigma F_{4,j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEreg$

5. service life

$RELEASEreg_{5,j}$:
air $F_{5,air} \cdot (1-\Sigma F_{3,j} - \Sigma F_{4,j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEreg$
water $F_{5,water} \cdot (1-\Sigma F_{3,j} - \Sigma F_{4,j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEreg$
soil $F_{5,ind} \cdot (1-\Sigma F_{3,j} - \Sigma F_{4,j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEreg$
surf $F_{5,surf} \cdot (1-\Sigma F_{3,j} - \Sigma F_{4,j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEreg$
total $\Sigma F_{5,j} \cdot (1-\Sigma F_{3,j} - \Sigma F_{4,j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEreg$

6. waste treatment

$RELEASEreg_{6,j}$:
air $F_{6,air} \cdot (1-\Sigma F_{3,j} - \Sigma F_{4,j} - \Sigma F_{5,j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEreg$
water $F_{6,water} \cdot (1-\Sigma F_{3,j} - \Sigma F_{4,j} - \Sigma F_{5,j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEreg$
soil $F_{6,ind} \cdot (1-\Sigma F_{3,j} - \Sigma F_{4,j} - \Sigma F_{5,j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEreg$
surf $F_{6,surf} \cdot (1-\Sigma F_{3,j} - \Sigma F_{4,j} - \Sigma F_{5,j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEreg$
total $\Sigma F_{6,j} \cdot (1-\Sigma F_{3,j} - \Sigma F_{4,j} - \Sigma F_{5,j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEreg$

Input

$F_{i,j}$	fraction of tonnage released during stage *i* to compartment *j*	[-]	O
PRODVOLreg	regional production volume of substance	$[kg_c.d^{-1}]$	O
TONNAGEreg	regional tonnage of substance	$[kg_c.d^{-1}]$	O

Output

$RELEASEreg_{i,j}$	regional release during life-cycle stage *i* to compartment *j*	$[kg_c.d^{-1}]$	O

III.3.3 Local emission rates: new and existing substances

For estimating local releases, point sources (and therefore, presumably, single stages of the life cycle) need to be identified. The main point sources are identified for each stage of the life cycle and each relevant application. Exception are intermediates (IC/UC=3/33) where emissions at production are added to emissions during industrial use (and production is set to zero) unless it is explicitly stated that the chemical is processed elsewhere. Each application and each relevant stage of the life cycle is assessed separately.

The emission rate is given as a release rate during an emission episode, and averaged per day (24 hours). It should be noted that in the emission scenario documents the emissions can be given in tonnes.yr^{-1}. In EUSES the output is calculated in kg d^{-1}.

III.3.3.1 Emissions based on tonnage with general B-tables (possibly updated with emission factors of emission scenario documents of the TGD)

$$Elocal_{i,j} = Fmainsource_i \cdot RELEASEreg_{i,j} \frac{365}{Temission_i} \quad j \in \{air,water\} \qquad (10)$$

III.3.3.1.1 IC 14 Paints, lacquer and varnished industry

Life cycle stage Formulation

$$Elocal_{2,j} = \frac{TONNAGEreg \cdot 10^3 \cdot Fmainsource_2 \cdot F_{2,j}}{Temission_2} \quad j \in \{air,water\} \qquad (11)$$

Input			
TONNAGEreg	relevant tonnage in the region for this application	[tonnes.yr^{-1}]	O
$Temission_i$	number of emission days per year	[d.yr^{-1}]	D
$Fmainsource_i$	fraction of the main local source	[-]	D
$F_{2,j}$	fraction of the tonnage released to compartment *j* during formulation	[-]	D, P
Output			
$Elocal_{2,water}$	local emission to wastewater	[kg$_c$.d^{-1}]	O
$Elocal_{2,air}$	local emission to air	[kg$_c$.d^{-1}]	O

Table III-3 *Defaults for emission calculations.*

Parameter	Symbol	Unit	Value
number of emission days per year	$Temission_2$	[d.yr^{-1}]	B-table$^{2)}$
fraction of the main local source	$Fmainsource_2$	[-]	B-table$^{2)}$
fraction of the tonnage released to compartment *j*	$F_{2,j}$	[-]	$^{1)}$

$^{1)}$ see pick-list Table III-4

$^{2)}$ Table B 2.3 for HPVC, Table 2.10 for non-HPVC

Table III-4 *Emission factors to air ($F_{2,air}$) and (waste)water ($F_{2,water}$) for formulation of various types of paint and coating products. I= volatile*[1]*, II = non-volatile & water soluble*[2] *and III = non-volatile & non-water soluble.*

Type of application/product	**I**		**II**		**III**	
	$F_{2,air}$	$F_{2,water}$	$F_{2,air}$	$F_{2,water}$	$F_{2,air}$	$F_{2,water}$
furniture	0.01	0.01	0	0.01	0	0.01
UV curable wood lacquer	0.02	0	0	0	0	0
water-borne wood lacquer	0.01	0.02	0	0.02	0	0.02
nitrocellulose wood lacquer (spray)	0.02	0	0	0	0	0
coil coating	0.01	0	0	0.01	0	0.01
can coatings (general)	0.03	0	0	0	0	0
solvent based 2 piece can external white enamel	0.018	0	0	0	0	0
water-borne 2 piece can external white enamel	0.015	0	0	0	0	0
epoxy-phenolic food-can lacquer (solvent-based)	0.015	0	0	0	0	0
general line varnish for metal cans (solvent-based)	0.015	0	0	0	0	0
general line white coating for metal cans (solvent-based)	0.02	0	0	0	0	0
solvent-based general purpose size (metal cans)	0.01	0	0	0	0	0
marine coatings	0.03	0	0	0	0	0
container coating	0.04	0	0	0	0	0
OEM car manufacturing	0.03	0	0	0	0	0
car refinish	0.03	0	0	0	0	0
vinyl matt emulsion	0.01	0	0	0.02	0	0
standard alkyd gloss finish	0.02	0	0	0.02	0	0.01
water-borne exterior woodstain	0.02	0.01	0	0.01	0	0.01
solvent-borne exterior/interior woodstain	0.01	0	0	0	0	0.01
Undefined/unknown	0.04	0.02	0	0.02	0	0.02

1) volatile substances are defined as having a vapour pressure of > 10 Pa at 23 °C

2) a substance is considered to be “water soluble” if its water solubility is > 1 $g.l^{-1}$

Life cycle stage Industrial use (i=3) and Private use (i=4)

$$Elocal_{i,j} = \frac{TONNAGEreg \cdot Fmainsource_i \cdot F_{i,j}}{Temission_i} \quad j \in \{air,water\} \quad (12)$$

Input

TONNAGEreg	relevant tonnage in the region for this application	$[kg_c.yr^{-1}]$	O
$Temission_i$	number of emission days per year	$[d.yr^{-1}]$	D
$Fmainsource_i$	fraction of the main local source	[-]	D
$F_{i,j}$	fraction of the tonnage released to compartment *j* during life cycle stage i	[-]	D, P

Output

$Elocal_{i,water}$	local emission to wastewater	$[kg_c.d^{-1}]$	O
$Elocal_{i,air}$	local emission to air	$[kg_c.d^{-1}]$	O

Table III-5 *Defaults for emission calculations.*

Parameter	**Symbol**	**Unit**	**Value**
number of emission days per year	$Temission_i$	$[d.yr^{-1}]$	B-table[2)]
fraction of the main local source	$Fmainsource_i$	[-]	B-table[2)]
fraction of the tonnage released to compartment *j*	$F_{i,j}$	[-]	[1)]

[1)] see pick-list ***Table III-6***

[2)] *i* = 3: Table B 3.13; *i* = 4: Table B 4.4 (for wastewater only)

Table III-6 *Emission factors to air ($F_{i,\ air}$) and (waste)water ($F_{i,\ water}$) for industrial use (i = 3) and private use (i = 4) of various types of paint and coating products. I= volatile[1)], II = non-volatile & water soluble[2)] and III = non-volatile & non-water soluble.*

Type of applicate ion / product	***i***	**I**		**II**		**III**	
		$F_{i,air}$	$F_{i,water}$	$F_{i,air}$	$F_{i,water}$	$F_{i,air}$	$F_{2,water}$
Furniture	4	0.97	0.01	0	0.03	0	0.03
UV curable wood lacquer	4	0.98	0	0	0	0	0
water-borne wood lacquer	4	0.92	0.05	0	0.05	0	0.05
nitrocellulose wood lacquer (spray)	4	0.98	0	0	0	0	0
coil coating	3	0.01	0.01	0	0.01	0	0.01
can coatings (general)	3	0.94	0	0	0	0	0
solvent based 2 piece can external white enamel	3	0.96	0	0	0	0	0
water-borne 2 piece can external white enamel	3	0.965	0	0	0	0	0
epoxy-phenolic food-can lacquer (solvent-based)	3	0.93	0	0	0	0	0
general line varnish for metal cans (solvent-based)	3	0.934	0	0	0	0	0
general line white coating for metal cans (solvent-based)	3	0.927	0	0	0	0	0
solvent-based general purpose size (metal cans)	3	0.939	0	0	0	0	0

marine coatings	4	0.97	0	0	0	0	0.05
container coating	4	0.96	0	0	0	0	0
OEM car manufacturing	3	0.97	0	0	0	0	0
car refinish	4	0.97	0	0	0	0	0.01
vinyl matt emulsion	4	0.96	0.01	0	0.03	0	0.03
standard alky~~d~~ gloss finish	4	0.96	0.01	0	0.03	0	0.03
water-borne exterior woodstain	4	0.96	0.01	0	0.02	0	0.02
solvent-borne exterior/interior woodstain	4	0.98	0.01	0	0	0	0.03
Undefined/unknown (industrial use)	3	0.98	0.05	0	0.05	0	0.05
Undefined/unknown (private use)	4	0.97	0.01	0	0.01	0	0.01

1) volatile substances are defined as having a vapour pressure of > 10 Pa at 23 °C

2) a substance is considered to be “water soluble” if its water solubility is > 1 $g.l^{-1}$

III.3.3.2 Emissions based on tonnage with ***specific B-tables*** *(derived from emission scenario documents)*

This calculation is performed for:

- IC 5 Personal/domestic and UC 9 and 15 (if production volume > 1000 tonnes/year) for private use ($i = 4$)
- IC 6 Public domain and UC 9 (if production volume > 1000 tonnes/year) for industrial use ($i = 3$)

The emissions in these scenarios are not included in the regional assessment (only local)

$$Elocal_{i,water} = \frac{TONNAGEreg \cdot Nlocal}{N \cdot Temission_i} \qquad (13)$$

Input

TONNAGEreg	regional tonnage of substance	$[kg_c.d^{-1}]$	O
Nlocal	number of inhabitants feeding one STP	[-]	D
N	number of inhabitants feeding regional system	[-]	D
$Temission_i$	number of days per year for emission in stage *i*	$[d.yr^{-1}]$	D

Output

$Elocal_{i,water}$	local emission to wastewater	$[kg_c.d^{-1}]$	O

III.3.3.3 Emission based on average capacities and consumptions (derived from emission scenario documents)

This calculation is performed for:

- IC 7 Leather processing industry for UC 10 Colouring agents and UC 51 Tanning agents at industrial use
- IC 8 Metal extraction industry, refining and processing industry and for UC 11 Complexing agents, UC 14 Corrosion inhibitors, UC 29 Heat transfer agents, UC 35 Lubricants and additives, UC 40 pH-regulating agents, UC 49 Stabilisers and UC 50 Surface-active agents at waste treatment
- IC-10 Photographic industry for UC 42 Photochemicals at industrial use and waste treatment (i.e., silver recovery process)
- IC 12 Pulp, paper and board industry and UC 2 adhesives and binding agents, UC 10 colouring agents, UC 31 Impregnation agents, UC 43, Process regulators, UC 47 softeners and UC 55 others
- IC 13 Textile processing industry UC 10 colouring agents
- IC 14 Paint, lacquers and varnished industry and UC 2 adhesives and binding agents, UC 48 solvents, UC 10 colouring agents, UC 20 fillers and UC 52 viscosity adjusters
- IC 11 Polymers industry and UC 53 vulcanising agents, UC 20 fillers, UC 49 stabilisers and UC 22 flame retardants and other UCs

These emissions in these scenarios are not included in the regional assessment (only local)

III.3.3.3.1 IC 7 Leather processing industry

UC 10 Dyes:

$$Elocal_{3,water} = Qleather \cdot Qsubst \cdot Fdye \cdot (1 - Ffix) \qquad (14)$$

Input

Qleather	quantity of treated raw hide per day	$[tonnes.d^{-1}]$	D
Qsubst	quantity of substance used per tonne of raw hide	$[kg_c.tonne^{-1}]$	D
Ffix	degree of fixation	[-]	D, P
Fdye	fraction of daily production dyed with on dye	[-]	D
Output			
$Elocal_{3,\ water}$	local emission to wastewater	$[kg_c.d^{-1}]$	O

Table III-7 *Defaults for emission calculations.*

Parameter	Symbol	Unit	Value
quantity of treated raw hide per day	Qleather	$[tonne.d^{-1}]$	15
quantity of substance used per tonne of raw hide	Fconc	$[kg.tonne^{-1}]$	10
degree of fixation for the dye types:	Ffix	[-]	
sulphur			0.70
metal complex			0.94
acid			1.00
unknown/acid groups			0.96
fraction of daily production dyed with one dye	Frel	[-]	0.50

UC 51 Tanning agents:

$$Elocal_{3,water} = Qleather \cdot Qsubst \cdot (1 - Ffix) \qquad (15)$$

Input

Qleather	quantity of treated raw hide per day	$[tonnes.d^{-1}]$	D
Qsubst	quantity of substance used per tonne of raw hide	$[kg_c tonne^{-1}]$	S
Ffix	degree of fixation	[-]	S
Output			
$Elocal_{3,water}$	local emission to wastewater	$[kg_c.d^{-1}]$	O

Table III-8 *Defaults for emission calculations.*

Parameter	Symbol	Unit	Value
quantity of treated raw hide per day	Qleather	$[tonne.d^{-1}]$	15

III.3.3.3.2 IC 8 Metal extraction industry, refining and processing industry

Life cycle stage Waste treatment

A) Water-based cooling lubricants

A.1) Cooling lubricant emulsions:

$$Cconc = Fconc \cdot RHOconc \tag{16}$$

$$Elocal_{6,water} = \frac{Fproc}{Fproc + 1} \cdot \frac{Cconc \cdot Vproc}{1 + Fproc \cdot K_{ow}} \cdot Frel \cdot (1 - Felim) \tag{17}$$

Input

Cconc	concentration of substance in concentrate	[$kg_c.m^{-3}$]	O
Fconc	fraction of substance in concentrate	[-]	S/P
RHOconc	density of the concentrate	[$kg_c.m^{-3}$]	D
Vproc	volume of processed liquid treated in recovery unit	[$m^3.d^{-1}$]	D
Fproc	fraction of concentrate in processed liquid	[-]	S/P
K_{ow}	octanol-water partition coefficient	[-]	S
Felim	fraction of the substance eliminated during treatment	[-]	D
Frel	factor of relevance	[-]	D
Output			
$Elocal_{6,\ water}$	local emission to wastewater	[$kg_c.d^{-1}$]	O

Table III-9 *Defaults for emission calculations.*

Parameter	Symbol	Unit	Value
Fraction of substance in concentrate	Fconc	[-]	1)
Density of concentrate	RHOconc	[$kg.m^{-3}$]	1000
Volume of processed liquid treated in recovery plant	Vproc	[$m^3.d^{-1}$]	40
Fraction of concentrate in processed liquid	Fproc	[-]	2)
Octanol-water partition coefficient	K_{ow}	[-]	3)
Fraction of the substance eliminated during treatment	Felim	[-]	0.8
Factor of relevance	Frel	[-]	1

1) see pick-list Table III-11

2) see pick-list Table III-12

3) substance specific property

A.2) water-soluble lubricants:

$$Cconc = Fconc \cdot RHOconc \tag{18}$$

$$Elocal_{6,water} = Cconc \cdot Vproc \cdot Fproc \cdot Frel \cdot (1 - Felim) \tag{19}$$

Input			
Cconc	concentration of substance in concentrate	$[kg_c.m^{-3}]$	O
Fconc	fraction of substance in concentrate	[-]	S/P
RHOprod	density of concentrate	$[kg.m^{-3}]$	D
Vproc	volume of processed liquid treated in recovery unit	$[m^3.d^{-1}]$	D
Fproc	fraction of concentrate in processed liquid	[-]	S/P
Felim	fraction of the substance eliminated during treatment	[-]	D
Frel	factor of relevance	[-]	D
Output			
$Elocal_{6,\ water}$	local emission to wastewater	$[kg_c.d^{-1}]$	O

Table III-10 *Defaults for emission calculations.*

Parameter	**Symbol**	**Unit**	**Value**
Fraction of substance in concentrate	Fconc	[-]	1)
Density of concentrate	RHOconc	$[kg.m^{-3}]$	1000
Volume of processed liquid treated in recovery plant	Vproc	$[m^3.d^{-1}]$	40
Fraction of concentrate in processed liquid	Fproc	[-]	2)
Fraction of the substance eliminated during treatment	Felim	[-]	0.8
Factor of relevance	Frel	[-]	1

1) see pick-list, Table III-11

2) see pick-list Table III-12

Table III-11 *Pick-list for the composition of cooling lubricants, with the fraction of the substance in concentrate, Fconc (-) and the use category (UC) if applicable. The highest concentration is used as a worst case in case of reported ranges (n.a. = not applicable).*

Substance group	**UC**	**traditional SEM**[1]	**synthetic SEM**[1]	**SES**[2]
base oil (lubricants)	35	0.60	0.30	n.a.
anti-wear additives	35	0.05	0.05	0.05
complex builders (complexing agents)	11	0.05	0.05	0.05
corrosion inhibitor (corrosion protection)	14	0.05	0.20-0.25	0.20-0.40
emulsifier:	49			n.a.
- anionic		0.15-0.2		
- not ionic			0.10-0.15	
- others/unknown		0.20	0.2	
extreme pressure additives	35	0.5	0.5	0.5
foam inhibitors	35	0.003	0.003	0.003
friction modifier	35	0-0.05	0.05-0.10	0.05-0.10
metal deactivators	35	0.01	0.01	0.01
pH-regulating agents (neutralisation agents)	40	0.03		0.25

solubilisers	35	0.05	0.05	0.10-0.20
surfactants:	50			
- anionic surfactants		0.25	0.25	0.25
- others/unknown		0.25	0.25	0.25

[1] SEM emulsifiable cooling lubricant

[2] SES water soluble cooling lubricant

Table III-12 *Pick-list for fraction of cooling lubricant concentrate in processed liquid, Fproc (-) by type of process. The highest concentration is used as a worst case when ranges are reported.*

Process	Fproc
Broaching	0.10-0.20
thread cutting	0.05-0.10
deep hole drilling	0.10-0.20
parting-off	0.05-0.10
milling, cylindrical milling	0.05-0.10
turning, drilling, automation work	0.03-0.10
Sawing	0.05-0.20
tool grinding	0.03-0.06
cylindrical grinding	0.02-0.05
centreless grinding	0.03-0.06
surface grinding	0.02-0.05

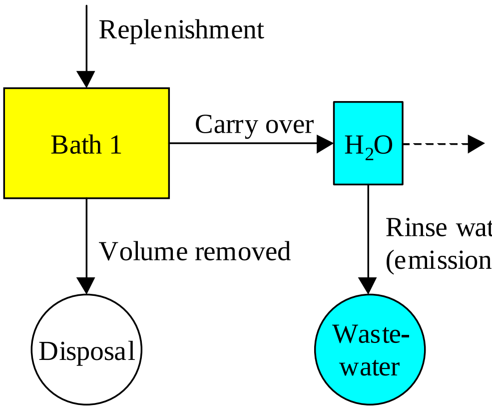
III.3.3.3.3 IC-10 Photographic industry and UC 42 Photochemicals

Life cycle stage Industrial use

Four typical point sources with photographic processes are considered:
- wholesale finisher
- large X-ray division at a hospital
- large printing office for reprographic activities
- copying facility

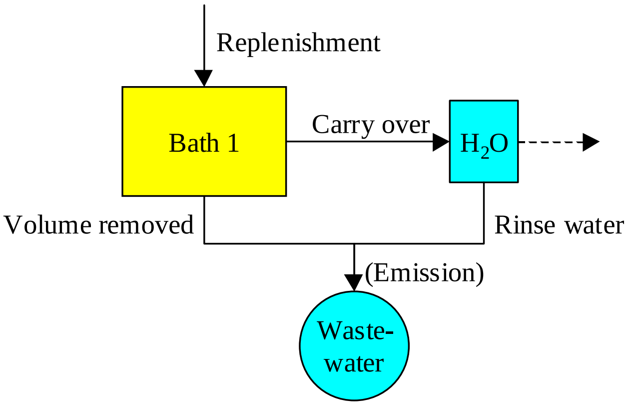
In respect to wastewater emissions the following situations are considered:

① Emissions to wastewater resulting from intermediate rinsing between the photochemical process baths where the substance is introduced and the next bath or final rinsing, if the volume removed from the bath is sent for recovery/treatment ("disposal") *(see diagram)*:



$$Elocal_{3,water} = Cform \cdot AREAmaterial \cdot Vcarry\_over \cdot (1-Fconv) \cdot 10^{-3} \qquad \textbf{(20)}$$

② Emissions to wastewater if the volume removed from the bath where the substance is introduced goes also directly to wastewater *(see also diagram)*:



$$Elocal_{3,water} = Cform \cdot AREAmaterial \cdot Vrepl \cdot (1-Fconv) \cdot 10^{-3} \qquad \textbf{(21)}$$

Input

Cform	concentration of substance in working solution	[$kg_c.m^{-3}$]	S/P
AREAmaterial	surface of processed film or paper	[$m^2.d^{-1}$]	S/P
Vrepl	replenishment rate	[$l.m^{-2}$]	S/P
Vcarry-over	carry-over rate	[$l.m^{-2}$]	S/P
Fconv	fraction of the substance removed or converted during process	[-]	D

Output

$Elocal_{3,\ water}$	local emission to wastewater	[$kg_c.d^{-1}$]	O

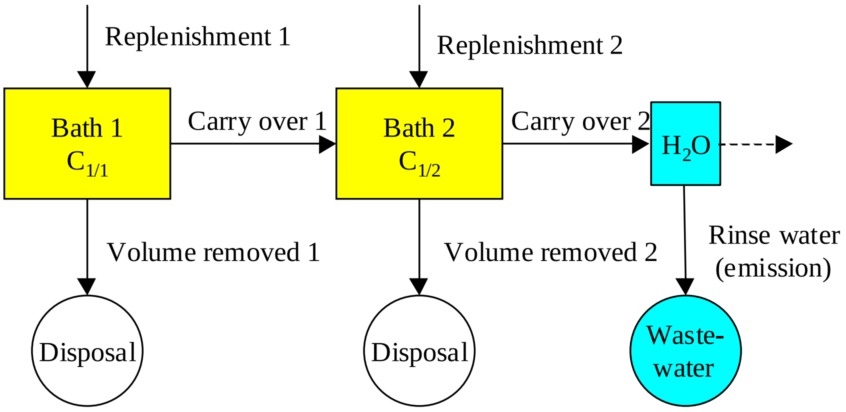
Table III-13 *Defaults for emission calculations.*

Parameter	**Symbol**	**Unit**	**Value**
concentration of substance in working solution	Cform	[$kg_c.m^{-3}$]	1)
surface of processed film or paper	AREAmaterial	[$m^2.d^{-1}$]	2)
replenishment rate	Vrepl	[$l.m^{-2}$]	2)
carry-over rate	Vcarry-over	[$l.m^{-2}$]	2)
fraction of substance removed or converted during process	Fconv	[-]	0

1) see pick-list Table III-18

2) see pick-list Table III-17

③ Emissions to wastewater when the carry-over of a processing bath, where the substance was entered goes to a next bath, which is followed by a washing step. The volumes removed from the baths are sent for recovery/treatment ("disposal") *(see also diagram)*:



$$Csubst_{1-2} = Cform_{bath\,1} \cdot \frac{Vcarry\_over}{Vcarry\_over + Vrepl_{bath\,2}} \qquad (22)$$

$$Elocal_{3,water} = Csubst_{1-2} \cdot AREAmaterial \cdot Vcarry\_over \cdot (1\text{-}Fconv) \cdot 10^{-3} \qquad (23)$$

Input

Csubst$_{1\text{-}2}$	concentration of substance from first bath in the second bath	$[kg_c.m^{-3}]$	O
Cform$_{bath\ 1}$	concentration of substance in working solution of bath one	$[kg_c.m^{-3}]$	S/P
AREAmaterial	surface area of processed film or paper	$[m^2.d^{-1}]$	S/P
Vrepl$_{bath\ 2}$	replenishment rate of second bath	$[l.m^{-2}]$	S/P
Vcarry-over	carry-over rate	$[l.m^{-2}]$	S/P
Fconv	fraction of the substance removed or converted during process	[-]	D

Output

Elocal$_{3,\ water}$	local emission to wastewater	$[kg_c.d^{-1}]$	O

Table III-14 *Defaults for emission calculations.*

Parameter	**Symbol**	**Unit**	**Value**
concentration of substance in first bath	Cform$_{bath\ 1}$	$[kg_c.m^{-3}]$	1)
surface of processed film or paper	AREAmaterial	$[m^2.d^{-1}]$	2)
replenishment rate	Vrepl	$[l.m^{-2}]$	2)
carry-over rate	Vcarry-over	$[l.m^{-2}]$	2)
fraction of substance removed or converted during process	Fconv	[-]	0

1) see pick-list Table III-18

2) see pick-list Table III-17

Release of substances from processing photographic materials:

$$Elocal_{3,water} = Qsubst \cdot AREAmaterial \cdot Fdiss \cdot \left(1 - Fconv\right) \tag{24}$$

Input

Qsubst	quantity of substance in the photographic material	$[kg_c.m^{-2}]$	S/P
AREAmaterial	surface area of processed film or paper	$[m^2.d^{-1}]$	S/P
Fdiss	fraction substance dissolved during processing	[-]	D
Fconv	fraction removed or converted during processing	[-]	D

Output

Elocal$_{3,\ water}$	local emission to wastewater	$[kg_c.d^{-1}]$	O

Table III-15 *Defaults for emission calculations.*

Parameter	**Symbol**	**Unit**	**Value**
Quantity of substance in the photographic material	Qsubst	$[kg_c.m^{-2}]$	1)
Surface area of processed film or paper	AREAmaterial	$[m^2]$	2)
fraction of substance removed or converted during process	Fconv	[-]	0
fraction which dissolves during processing	Fdiss	[-]	1

1) see pick-list Table III-20

2) see pick-list Table III-17

Life cycle stage Waste treatment

Release at the disposal company:

$$Elocal_{6,water} = Cform \cdot Vtreat \cdot \left(1 - Fconv\right) \cdot \left(1 - Fred\right) \tag{25}$$

Input			
Cform	concentration of substance in the fresh working solution	[$kg_c.m^{-3}$]	P
Vtreat	treated volume of working solution	[$m^3.d^{-1}$]	P
Fconv	fraction of the substance removed or converted during process	[-]	D
Fred	fraction of waste reduction	[-]	D
Output			
$Elocal_{6,\ water}$	local emission to wastewater	[$kg_c.d^{-1}$]	O

Table III-16 *Defaults for emission calculations.*

Parameter	**Symbol**	**Unit**	**Value**
concentration of substance in working solution	Cform	[$kg_c.m^{-3}$]	1)
treated volume of working solution	Vtreat	[m^3]	2)
fraction of substance removed or converted during process	Fconv	[-]	0
fraction of waste reduction	Fred	[-]	0

1) see pick-list Table III-18

2) see pick-list Table III-19

Table III-17 *Pick-list for release estimation parameters replenish rate, Vrepl ($l.m^{-2}$), carry-over rate, Vcarry-over ($l.m^{-2}$) and treated area of photographic material, AREAmaterial ($m^2.d^{-1}$). When there is no intermediate washing step the replenish rate is set to the lowest value. At direct introduction into wastewater the replenish rate is set to the highest value as worst case.*

Process[a]	**Bath**	**Vrepl**[b]	**Vcarry-over**	**AREAmaterial**
wholesale finisher				
C-41				
colour negative	developing	0.30–0.60 (0.45)	0.080 / 0.170[c]	680
	bleaching	0.10–0.90 (0.50)		
	fixing	0.40–0.90 (0.65)		
	stabilising	0.90 (0.90)		
RA-4				
colour paper	developing	0.06–0.12 (0.09)	0.040 / 0.070[c]	4950
	bleach fixing	0.07–0.14 (0.10)		
RA-4				
devided bleaching and fixing	developing	0.06–0.12 (0.09)	0.050	
	stopping	0.15–0.20 (0.175)		
	bleaching	0.05–0.10 (0.075)		
	fixing	0.055–0.100 (0.075)		
	stabilising			
E-6				
colour reversal film	primary developing	0.9–1.8 (1.35)	0.080 / 0.170[c]	120
	reversing	1.0–1.1 (1.05)		
	colour developing	1.0–2.0 (1.5)		
	conditioning	0.9–1.1 (1.0)		
	bleaching	0.2 (0.2)		
	fixing	0.4–1.0 (1.2)		
	stabilising	1.0 9(1.0)		
R-3				
colour reversal paper	primary developing	0.17–0.33 (0.25)	0.050	350
	colour developing	0.05–0.50 (0.275)		
	bleach fixing	0.07–0.20 (0.135)		
	stabilising			
R-3				
devided	primary developing	0.17–0.33 (0.25)		

Process[a]	**Bath**	**Vrepl**[b]	**Vcarry-over**	**AREAmaterial**
bleaching and fixing	colour developing	0.05-0.50 (0.275)		
	bleaching	0.07–0.14 (0.105)		
	fixing	0.055-0.100 (0.775)		
	stabilising			
BW-N				
	developing	0.5-0.6 (0.55)	0.180	40
	fixing	0.4-0.9 (0.65)		
BW-P				
	developing	0.2-0.3 (0.25)	0.070	270
	fixing	0.055-0.30 (0.178)		
x-ray division				
BW-X				
med.	developing	0.35-0.40 (0.375)	0.040	110
	fixing	0.4-0.6 (0.50)		
BW-X				
tech.	developing	0.5-0.6 (0.55)	0.040	
	fixing	0.8-1.2 (0.10)		
printing office				
BW-R				
film	developing	0.2-0.3 (0.25)	0.040	80
	fixing	0.15-0.30 (0.225)		
copy facility				
ECN-2				
cine- and television-film negative	primary bath	0.375	0.180	35
	colour developing	0.845		
	stopping	0.560		
	bleach accelerating	0.180		
	bleaching	0.180		
	fixing	0.560		
	stabilising	0.375		
ECP-2				
cine- and television positive	primary bath	0.374	0.180	350
	colour developing	0.646		
	stopping	0.721		
	primary fixing	0.187		
	bleach accelerating	0.187		
	bleaching	0.187		
	secondary fixing	0.187		
	stabilising	0.374		
VNF-1				
cine- and television-film reversal	primary developing	0.348	0.180	35
	primary stopping	2.254		
	colour developing	1.639		
	secondary stopping	1.332		
	bleach accelerating	0.410		
	bleaching	0.410		
	fixing	1.281		
	stabilising	0.615		

a values of C-41, RA-4, E6, R-3, BW-P and BW-N are related to point source (a) -wholesale finisher
values of BW-X are related to point source (b) –hospital
values of BW-R are related to point source (c) -printing office
values of ECN-2, ECP-2 and VNF-1 are related to point source (d) –copying facility

b recycling processes of bath-solutions for point source (a) –wholesale finisher- are considered

c carry-over rates for professional labs are different from wholesale finishers

Table III-18 *Pick-list for the content of substance in processing solutions for every specific function, Cform (kg$_c$.m^{-3}), and the corresponding equation (Eq = equation, Dev = developer, pH-reg = pH regulator, Antiox = antioxidant, Antifog = antifogging agent, Bleach = bleaching agent, Rehalog = rehalogenating agent, Fix = fixing agent, Stab = stabiliser, Seq = sequestering agent, Rev = reversing agent, Hard = hardening agent, Solv = auxiliary solvent, and Bl Acc = bleaching accelerator*

Process	**Process bath**	**Eq**	**Dev**	**pH-reg**	**Antiox**	**Antifog**	**Bleach**	**Rehalog**	**Fix**	**Stab**	**Seq**	**Rev**	**Hard**	**Solv**	**Bl Acc**
UC			**42**	**40**	**49**	**42**	**8**	**42**	**21**	**49**	**11**	**42**	**55/0**	**48**	**43**
Wholesale finisher															
C-41	Developing	3 (n=2)	8	50	6	2					4			19	
	Bleaching	1		20			120	120							0.4
	Fixing	1		20	8				150						
	Stabilising	2								2					
RA-4	Developing	1	8	40	8	1.6					4			19	
	Stopping	1													
	Bleaching	1		10			50	52.5							0.4
	Fixing	1			10				90		3				
E-6	Primary developing	1	30	35	6.5	2					4			19	
	Reversing	3 (n=2)										2			
	Colour developing	1	10	50	6	1.6					4			19	
	Conditioning	2		20											
	Bleaching	3 (n=2)					150	80							0.4
	Fixing	1			8				180						
	Stabilising	2								2					
R-3	Primary developing	1	20	30	2	1.6					4	4		19	
	Colour developing	1	7	30	6.5	1.6					4	4		19	
	Bleach fixing	1		20	10		60		100						
	Stabilising	1								2					
BW-N	Developing	1	15	70	20	10					10				
	Fixing	1		20	20				150				5		
BW-P	Developing	1	15	70	20	10					10				
	Fixing	1		20	20				150				5		
Printing office															
BW-R	Developing	1	25	20	8	17					10				
	Fixing	1		15	15				120						

Process	**Process bath**	**Eq**	**Dev**	**PH-reg**	**Antiox**	**Antifog**	**Bleach**	**Rehalog**	**Fix**	**Stab**	**Seq**	**Rev**	**Hard**	**Solv**	**Bl Acc**
UC			**42**	**40**	**49**	**42**	**8**	**42**	**21**	**49**	**11**	**42**	**55/0**	**48**	**43**
X-ray division															
BW-X	Developing	1	20	60	20	17					10				
	Fixing	1		20	20				150						
Copying facility															
ECN-2	Primary bath	3 (n=3)		0.8	55.6										
	Colour developing	3 (n=2)	3	13.5	1.4	0.43					4			19	
	Stopping	1				26.3									
	Bleach accelerating	1		15.8	6.3										0.4
	Bleaching	1		8.5		30.4	80	120							
	Secondary fixing	1			12.9				68.2						
	Stabilising	1								8					
ECP-2	Primary bath	3 (n=3)		0.8									55.6		
	Colour developing	3 (n=2)	11.5	9.5	2.4	0.8					4			19	
	Stopping	1				26.3									
	Primary fixing	1			8.9	0.4			54.8						
	Bleach accelerating	1		3.7	2.9										0.4
	Bleaching	1					13.7	120							
	Secondary fixing	1			8.9	0.4			54.8						
	Stabilising	1								1.95					
VNF-1	Primary developing	1	0.2	16.1	1.6	0.004			0.8	0.1	4			19	
	Primary stopping	1		16.7											
	Colour developing	1	6.7	2.6	4.3	0.02				0.06	4			19	
	Secondary stopping	1		16.7											
	Bleach accelerating	3 (n=3)		4.4	5.6										0.4
	Bleaching	3 (n=2)					47.2	120							
	Fixing	1			5.2				93.9						
	Stabilising	1								2					

N.B.
- ◘ If a specific bath is not mentioned the worst case default value for the substance with the specified function is used
- ◘ If the specific process for the photographic point source is not mentioned the worst case situation is used
- ◘ If the specific point source is not mentioned the worst case situation is used

Table III-19 *Pick-list for treated volume of working solution, Vtreat ($m^3.d^{-1}$) at the disposal company.*

Point source	**Photographic process**	**Treated volume**
If specific photographic process in unknown		
	colour process	3.0
	developing	1.0
	bleaching	0.3
	fixing	0.5
	bleach fixing	1.2
	black/white process	5.0
	developing	2.3
	fixing	2.7
If specific photographic process is known		
Whole sale finisher		
C-41	colour negative film	0.2
	developing	0.08
	bleaching	0.08
	fixing	0.04
RA-4	colour positive paper	2.6
	developing	0.78
	bleaching	0.21
	fixing	0.47
	bleach fixing	1.14
E-6	colour reversal film	0.03
	primary developing	0.013
	colour developing	0.013
	bleaching	0.003
	fixing	0.001
R-3	colour reversal paper	0.03
	primary developing	0.019
	colour developing	0.007
	bleach fixing	0.002
	bleaching	0.002
	fixing	0.001
BW-N	black/white negative film	0.06
	developing	0.05
	fixing	0.01
BW-P	black/white positive paper	0.18
	developing	0.16
	fixing	0.02
X-ray division		
BW-X	black/white X-ray	3
	developing	1.2
	fixing	1.8
Printing office		
BW-R	black/white reprographic	1.8
	developing	0.9
	fixing	0.9
	activator	
Copy facility		
Cine	cine- and television film	0.1
	developing	
	bleaching	

Table III-20 *Pick-list for content of substance in photographic material, Qsubst (kg.m^{-2}), which is released from the material in processing and cleaning solutions during processing of this material.*

Ingredient	**Paper**	**Film**
sensitizers	$1.0.10^{-6}$	$2.5.10^{-5}$
photographic stabilisers	$5.0.10^{-6}$	$1.0.10^{-4}$
fungicides	$3.0.10^{-5}$	$1.5.10^{-4}$
silver as Ag	$5.0.10^{-4}$	$1.2.10^{-2}$
halides	$3.0.10^{-4}$	$7.0.10^{-3}$
split-off products		
- masking compounds in negative films	$4.0.10^{-5}$	$8.0.10^{-5}$
- remaining groups of colour couplers	$8.0.10^{-5}$	$8.0.10^{-4}$
- stabilisers	0	$8.0.10^{-5}$
wetting agents	$1.0.10^{-5}$	$3.0.10^{-4}$
filter dyestuffs	$5.0.10^{-5}$	$2.5.10^{-4}$

III.3.3.3.4 IC 11 Polymers industry

Manufacture of rubber products (formulation and processing)

$$\boldsymbol{Elocal_{3,water} = Qrubber \cdot Qsubst \cdot (1 - Ffix)} \qquad \textbf{(26)}$$

Input			
Qrubber	amount of rubber product produced per day	[kg.d^{-1}]	D
Qsubst	amount of substance per unit of mass of product	[-]	P
Ffix	fraction of the substance remaining in the product	[-]	P
Output			
$Elocal_{3,\ water}$	local emission to wastewater	[kg$_c$.d^{-1}]	O

Table III-21 *Defaults for emission calculations.*

Parameter	**Symbol**	**Unit**	**Value**
amount of rubber product produced per day	Qrubber	[kg.d^{-1}]	55 000
amount of substance per unit of mass of product	Qsubst	[-]	1)
fraction of the substance remaining in the product	Ffix	[-]	1)

1) see pick-list Table III-22

Table III-22 *Pick-list for contents of rubber additives, Qsubst (-) in tyres and rubber products and the fractions remaining in the product, Ffix (-). When ranges are presented the highest value is chosen to represent the worst case situation.*

Parameter	**UC**	**rubber prod.**	**tires**	**Ffix**
mastication agents/ peptisers	**43**	**0.005 NR** **0.03 SR**	**0.005**	**0.995**
activators	46		0.02	
vulcanising agents		**0.0025 soft** **0.2 hard**	**0.01**	**1.000**
sulphur containing cross-linking agents	53	0.01	0.01	
vulcanising accelerators	43	0.0005-0.01	0.002-0.02	
accelerator activators	43	0.0075-0.025	0.0065	
sulphur-free cross-linking agents	53	0.000005-0.005	.	
co-agents for sulphur-free cross-linking agents	43	0.0025-0.01	0.01	
other cross-linking agents	53	0.000005-0.01	0.000005-0.01	
vulcanising retarders	43	0.0075-0.01	0.0015-0.01	
scorch-inhibitors	43	0.0005-0.005	0.0025	
anti-aging and antiflex-cracking agents/ anti-degradants		**0.004**	**0.004**	**0.98 RP** **0.99 TI**
antioxidants	49	0-0.015	0.0013	
antifatigue agents	49	0.005-0.025	0.001	

Parameter	**UC**	**rubber prod.**	**tires**	**Ffix**
anti-ozonants	49	0.005-0.035	0.001-0.005	
light protection agent	49	0-0.015	0.001	
anti-hydrolysis agents	49	0.0025-0.015	0.001	
heat protection agents	49	0.0025-0.015	0.005	
agents against metal poisoning	49	0.0025-0.015	0.001	
deactivators	49	0.0025	0.0015	
reversion protection agents	49	0.0025-0.015	.	
anti-cyclisation agents	49	0.0025	.	
quenchers	49	0.0025	.	
other anti-aging agents	49	0.0075-0.015	.	
fillers and pigments		**0.15**	**0.20**	**0.99**
fillers	20	0.05-0.15	0.20	
pigments	10	0.005-0.025	.	
plasticisers		**0.10**	**0.019**	**0.95**
natural plasticisers	47	0.05-0.10	0.012-0.019	
synthetic plasticisers	47	0.05-0.10	0.012-0.019	
processing aids		**0.075**	**0.005-0.025**	**0.995**
lubricants and flow improvers	35	0.025-0.075	.	
tackifiers	2	0.025-0.075	.	
factices		0.025-0.075	.	
filler activator	43	0.025-0.075	.	
blowing agents	25	0.025-0.05	0.015	1
bonding agents	2	0.005-0.02	0.015-0.02	1
stabilisers	49	0.0075-0.015	0.0075-0.015	
other agents		**0.0005-0.015**	**0.0005-0.015**	**0.95**
anti-cyclisation agents	49	.	.	
replastication agents	47	.	.	
emulsifier	49	0.0005-0.0025	.	
flame retardants	22	0.01-0.015	.	
solvents	48	.	.	
surface treatment agents	0/55	0.01-0.0215	0.01	
hardeners	0/55	.	.	
odour agents	36	0.000125-0.0005	.	
anti-static agents	7	0.001-0.003	0.025	
reinforcing agents	13	.	.	

Parameter	**UC**	**rubber prod.**	**tires**	**Ffix**
homogenisers	49	.	.	
latex-chemicals		**0.025**	**.**	**0.95 RP**
dispersion agents	43	0.005-0.01	.	
emulsifiers	49	0.005-0.025	.	
stabilisers	49	0.005-0.01	.	
wetting and foaming agents	50	0.005-0.01	.	
foam stabilisers	0/55	0.005-0.025	.	
thickeners	52	.	.	
coagulation agents	43	.	.	
vulcanisation agents	53	0.0025-0.01	.	
anti-aging chemicals	49	.	.	
fillers	20	.	.	
plasticisers	47	.	.	
release agents		**0.15**	**0.15**	**0.95**
release agents for unvulcanized rubber	0/55	0.0025-0.025	0.0025-0.025	
mould release agents	0/55	0.025-0.15	0.025-0.15	
mandrel release agents	0/55	0.025-0.15	0.025-0.15	
others		0.025	0.025	0.95
cleaning agents	9	.	.	
other rubber chemicals	0/55	.	.	

NR = natural rubber, SR = synthetic rubber, RP = rubber products, TI = tyres, hard = hard rubber, soft = soft rubber,
.=no data

III.3.3.3.5 IC 12 Pulp, paper and board industry

Emissions to surface water of chemicals used in the manufacture of paper (including coating of paper) and recycling of paper.

Life cycle stage Industrial use, Paper production

applied amount per ton of paper:

$$Elocal_{3,water} = Qsubst \cdot Qpaper \cdot (1 - Ffix) \cdot (1 - Fclosure) \qquad (27)$$

Input

Qsubst	consumption of substance per tonne of paper	[$kg_c.tonne^{-1}$]	S/P
Qpaper	quantity of paper produced on one site per day	[$tonnes.d^{-1}$]	P
Ffix	degree of fixation	[-]	S/P
Fclosure	degree of closure of the water system	[-]	P
Output			
$Elocal_{3,\ water}$	local emission to wastewater	[$kg_c.d^{-1}$]	O

***Table III-23** Defaults for emission calculations*

Parameter	Symbol	Unit	Value
consumption of substance per tonne of paper	Qsubst	[$kg_c.tonne^{-1}$]	1)
quantity of paper produced on one site per day	Qpaper	[$tonne.d^{-1}$]	2)
degree of fixation	Ffix	[-]	3)
degree of closure of the water system	Fclosure	[-]	2)

1) see pick-lists Table III-26 and Table III-27

2) see pick-list Table III-25

3) see pick-lists Table III-26 and Table III-28

Estimation if concentration of the substance in process water is used:

$$Elocal_{3,water} = Csubst \cdot Qwater \cdot Qpaper \cdot (1 - Ffix) \qquad (28)$$

Input

Csubst	concentration of substance in process water	[$kg_c.m^{-3}$]	S/P
Qwater	quantity of water used per tonne of paper	[$m^3.tonne^{-1}$]	P
Qpaper	quantity of paper produced on one site per day	[$tonne.d^{-1}$]	P
Ffix	degree of fixation	[-]	S/P
Output			
$Elocal_{3,water}$	local emission to wastewater	[$kg_c.d^{-1}$]	O

Table III-24 *Defaults for emission calculations.*

Parameter	**Symbol**	**Unit**	**Value**
concentration of substance in process water	Csubst	[$kg_c.m^{-3}$]	[1)]
quantity of water used per tonne of paper	Qwater	[$m^3.tonne^{-1}$]	[2)]
quantity of paper produced on one site per day	Qpaper	[$tonne.d^{-1}$]	[2)]
degree of fixation	Ffix	[-]	[1)]

[1)] see pick-list Table III-26

[2)] see pick-list Table III-25

Table III-25 *Pick-list for water consumption, Qwater ($m^3.tonne^{-1}$) degree of closure, Fclosure (-) and quantity of paper produced, Qpaper ($tonne.d^{-1}$) for various types of paper. In case of ranges the highest values for water consumption and quantity of paper produced are chosen as worst case. For degree of closure the lowest value is set as worst case.*

Type of paper produced	**Water consumption**	**Degree of closure**	**Quantity of paper produced**
printing and writing	40-75	0.40-0.70	100-1000
tissue	57	0.40-0.70	40-200
newsprint	24-35	0.65-0.85	100-1000
packaging and board	2-20	>0.95	100-1000

Table III-26 *Pick-list for amount of substance consumed per tonne, Qsubst (kg.tonne^{-1}) and degree of fixation, Ffix (-) for different types of substances used. For a worst case situation the highest value for the quantity of substance used and the lowest fixation rate are used.*

Type of substance used	**UC**	**Quantity of substance used, Qsubst [kg.tonne^{-1}]**				**degree of fixation**
		news paper	board	printing writing	tissue	**Ffix [-]**
charge control	43	0.2-1	0.3	0.03	0.03	0.7-0.9
retention aid	43	1-5	1-5			0.7-0.9
retention aid and strenght resin	43		20-30		2-12.5	0.7-0.9
softening	47			2-3		0.60-0.75
sizing agents	31					
natural (e.g. aluminumrosin)		4-10	4-10			0.10-0.30
synthetic						
(AKD =alkylketene dimers)				0.5-3		0.70-0.90
binding agent	2					.
starch		5-15	5-15			
CMC (carboxy methyl cellulose)		5-10				
surface coating	55/0	1-8	.			.
(e.g. wax, pur pigmented coating)						
Concentration in process water [kg.m^{-3}]						
anti-foaming	43	0.0002				.

Table III-27 *Pick-list for applied amount of dye (UC 10) , Qsubst (kg.tonne^{-1}) for various shades and types of paper. The highest value is chosen as a worst case situation.*

degree of shade	news paper	board	printing wrinting	tissue
pale shade			0.1-1	0.1-1
medium shade			1-10	1-10
deep shade			-	10-40

Table III-28 *Pick-list for degree of fixation, Ffix (-) for different types of dyes (UC 10) .The lowest values is chosen as a worst case situation.*

type of dye	**substrate**	**Degree of fixation [-]**
anionic direct	bleached and unbleached	0.79-0.90 0.98 with fixing agent
cationic direct	all types	0.90-0.99
Basic	bleached pulp mechanical pulp	0.50-0.70 0.60-0.80 0.95 with fixing agent
Acid	sized packaging paper	0.40-0.60 0.80-0.90 with fixing agent

Life cycle stage Waste treatment

Release during de-inking process:

$$\boldsymbol{TONNAGEreg = Fprodvol_{reg} \cdot TONNAGE} \qquad \textbf{(29)}$$

$$Elocal_{6,water} = \frac{TONNAGEreg \cdot Frec \cdot Fmainsource \cdot Fde-ink \cdot \left(1 - Fremoval\right) \cdot 10^3}{Temission_6} \qquad \textbf{(30)}$$

Input

$Fprodvol_{reg}$	fraction of the region	[-]	D
TONNNAGE	relevant tonnage in the EU for this substance	[$tonne.yr^{-1}$]	S
TONNAGEreg	relevant tonnage in the region for this substance	[$tonne.yr^{-1}$]	O
$Temission_6$	number of working days	[$d.yr^{-1}$]	D
Frec	rate of recycling (recycling fraction)	[-]	D
Fmainsource	fraction of the main source	[-]	D
Fde-ink	fraction released at de-inking	[-]	P
Fremoval	removal rate at on-site primary treatment	[-]	D
Output			
$Elocal_{6,\ water}$	local emission to wastewater	[$kg_c.d^{-1}$]	O

Table III-29 *Defaults for emission calculations.*

Parameter	**Symbol**	**Unit**	**Value**
Fraction of the region	$Fprodvol_{reg}$	[$kg_c.tonne^{-1}$]	$0.1^{1)}$
Number of paper production days	$Temission_6$	[$d.yr^{-1}$]	250
Fraction of the main sources	Fmainsource	[-]	0.10
Recycling rate	Frec	[-]	0.5

fraction released at de-inking	Fde-ink	[-]	2)
removal rate at on-site primary treatment	Fremoval	[-]	
- easily soluble (> 1000 $mg.l^{-1}$)			0.2
- insoluble (≤ 1000 $mg.l^{-1}$)			0.9

[1] for new substances or existing substances produced at low volumes and which are not used homogeneously throughout the EU, it can be assumed in a first approach that $Fprodvol_{reg}$ = 1

[2] see pick-list Table III-30 or Table III-31

Table III-30 *Fraction of ink released at de-inking process, Fde-ink (-) for various types of ink. Highest fraction of de-inking is used as a worst case value.*

Type of ink	**Fde-ink [-]**
mineral oil based	0.14-0.28
flexographic	0.30-0.90
non-impact toners	0.06-0.28

Table III-31 *Fraction of ink released at de-inking process, Fde-ink (-) for various ink drying processes. Highest fraction released at de-inking is used as a worst case value.*

method of ink drying	**Fde-ink [-]**
absorption, penetration, evaporation	0-0.20
oxidation or IR radiation	0.05-0.40
hot polymerisation or UV-fixation	0.10-0.60
ink-jet, laser or xerographic copying	0.40-0.70

III.3.3.3.6 IC 13 Textile processing industry

Life cycle stage Industrial use

Releases during wet processing:

UC 10 dyeing

$$Elocal_{3,water} = Qfibres \cdot Fdye \cdot Qform \cdot Fsubst \cdot (1 - Ffix) \qquad (31)$$

Input			
Qfibres	quantity of fibres / fabrics per day	[tonne.d^{-1}]	P
Fdye	fraction of fabric dyed with one dyestuff per day	[-]	D
Qform	quantity of dye-stuff formulation used on fabric	[kg.tonne^{-1}]	D/S
Fsubst	content of dye in the formulation	[kg$_c$.kg^{-1}]	D/S
Ffix	degree of fixation	[-]	P
Output			
Elocal$_{3, water}$	local emission to wastewater	[kg$_c$.d^{-1}]	O

Table III-32 Defaults for emission calculations.

Parameter	Symbol	Unit	Value
quantity of fibres / fabric treated per day	Qfibres	[tonne.d^{-1}]	1)
fraction of fabric dyed with one dye-stuff per day	Fdye	[-]	0.3
quantity of dye-stuff formulation used on fabric	Qform	[kg.tonne^{-1}]	10 2)
content of dye in the dye-stuff formulation	Fsubst	[kg$_c$.kg^{-1}]	1 3)
degree of fixation	Ffix	[-]	4)

1) see pick-list Table III-33

2) if no specific data are available, it should be assumed that the average mass of dye-stuff preparation used is 10 kg per tonne of fabric (1%)

3) if the content of dye-stuff in the preparation is not available, it should be assumed to be 100% (Fsubst = 1)

4) see pick-list Table III-34

Table III-33 Pick-list for daily production volumes, Qfibres (tonne.d^{-1}) at the textile production site.

Textile finishing company	Qfibres
Companies total (generic)	12.8
Dyeing	14.2
finishing cotton	23.2
finishing natural fibres	18.8
finishing synthetic fibres	5.8
finishing polyester fibres	0.8
using optical brightners	12.2

Table III-34 *Pick-list for degree of fixation, Ffix (-) for various types of dyes, dyeing processes and fibres.*

Dye	**Process**	**Fibre**	**Ffix**
disperse	continuous	cellulose and polyester	0.95
disperse	printing		0.97
direct	batch	cotton	0.88
reactive	batch	wool	0.95
reactive	batch	cotton	0.70
reactive	batch	general	0.85
vat	continuous	cotton	0.80
vat	printing		0.75
sulphur	continuous	cotton	0.70
sulphur	printing		0.70
acid, one SO_3-group	batch	polyamide and polyacryl	0.90
acid, more than one SO_3-group	batch		0.95
basic	batch	polyacryl, polyester, polyamide and cotton	0.99
azoic (naphtol)	continuous		0.84
azoic (naphtol)	printing		0.87
metal complex	batch		0.94
pigment	continuous		1.00
pigment	printing		1.00
unknown / hardly soluble	continuous		0.97
unknown / acid groups	printing		0.96

Finishing

$$Elocal_{3,water} = Qfibres \cdot Qform \cdot Fsubst \cdot (1 - Ffix) \tag{32}$$

Input

Qfibres	quantity of fibres / fabrics per day	[tonnes.d^{-1}]	P
Qform	quantity of formulation used on fabric	[kg.tonne^{-1}]	S
Fsubst	content of substance in the applied formulation	[kg$_c$.kg^{-1}]	D/S
Ffix	degree of fixation	[-]	D/S
Output			
$Elocal_{3,water}$	local emission to wastewater	[kg$_c$.d^{-1}]	O

Table III-35 *Defaults for emission calculations.*

Parameter	**Symbol**	**Unit**	**Value**
quantity of fibres / fabric treated per day	Qfibres	$[\text{tonne.d}^{-1}]$	[1]
quantity of formulation used on fabric	Qform	$[\text{kg.tonne}^{-1}]$	-
content of substance in the applied formulation	Fsubst	$[\text{kg}_c.\text{kg}^{-1}]$	1[2]
degree of fixation	Ffix	[-]	0

[1] see pick-list Table III-33

[2] if the content of the substance in the preparation is not available, it should be assumed to be 100%

Life cycle stage Service life

The release to wastewater (STP) is calculated as:

$$\boldsymbol{RELEASEreg_{k,5,water} = \frac{Fprodvol_{reg} \cdot F_{5,water} \cdot Qsubst\_tot_k \cdot 10^3 \cdot \sum_{y=1}^{Tservice_k} (1 - F_{5,water})^{y-1}}{Temission_5}} \qquad \textbf{(33)}$$

$$RELEASEreg_{5,water} = \sum_{k=1}^{m} RELEASEreg_{k,5,water} \qquad \textbf{(34)}$$

$$Elocal_{5,water} = Fmainsource_5 \cdot RELEASEreg_{5,water} \qquad \textbf{(35)}$$

Input

$Qsubst\_tot_k$	annual input of the substance in article *k*	$[\text{tonnes.yr}^{-1}]$	S
$Fprodvol_{reg}$	fraction of EU volume for region	[-]	D
$Tservice_k$	service life of article *k*	[yr]	P
$F_{5,water}$	fraction of the tonnage release over one year during the service to waste water	[-]	S
$Temission_5$	number of emission days per year	$[\text{d.yr}^{-1}]$	D
$Fmainsource_5$	fraction of the main source (STP)	[-]	D
$RELEASEreg_{k,5,water}$	release to waste water for article *k*	$[\text{kg}_c.\text{d}^{-1}]$	O
$RELEASEreg_{5,water}$	release to waste water for all articles	$[\text{kg}_c.\text{d}^{-1}]$	O

Output

$Elocal_{5, water}$	local emission to wastewater	$[\text{kg}_c.\text{d}^{-1}]$	O

Table III-36 *Defaults for emission calculations.*

Parameter	**Symbol**	**Unit**	**Value**
annual input of the substance in article k	$Qsubst\_tot_k$	[tonnes.yr^{-1}]	
fraction of EU volume for region	$Fprodvol_{reg}$	[-]	0.1
service life of article k	$Tservice_k$	[yr]	1)
fraction of the tonnage released over one year during service life	$F_{5,water}$	[-]	
number of emission days per year	$Temission_5$	[d.yr^{-1}]	365
fraction of the main source (STP)	$Fmainsource_5$	[-]	0.002

1) see pick-list Table III-37

Table III-37 *Service life of some article, Tservice$_k$ (yr). Some values are averages of the ranges presented in the emission scenario document.*

Article	**Service life**
clothes on contact with skin	1.0
other clothes and bed linen	3.5
household linen	7.5
Bedding	5.0
Carpets	14.0
wall-to-wall carpet	17.5
Sunblind	11.5
Tents	12.5
Awning	2.0

III.3.4 Regional emission rates

For the regional-scale assessments, the releases for each relevant application and stage of the life cycle must be summed into one emission for each compartment. The emissions are assumed to be a constant and continuous flux during the year. Of the emissions to water, part is directed to sewage treatment plants (STP).

$$Ereg_j = \sum_{i=1}^{5} RELEASEreg_{i,j} \qquad j \in \{air, ind\} \tag{36}$$

$$Ereg_{water} = Fconnect_{stp} \cdot \sum_{i=1}^{5} RELEASEreg_{i,water} \tag{37}$$

$$Ereg_{direct\text{-}water} = RELEASEreg_{i,surf} + (1 - Fconnect_{stp}) \cdot \sum_{i=1}^{5} RELEASEreg_{i,water} \tag{38}$$

Input			
$RELEASEreg_{i,j}$	regional release during life-cycle stage *i* to compartment *j*	$[kg_c.d^{-1}]$	O
$Fconnect_{stp}$	fraction connected to sewer systems	[-]	D
Output			
$Ereg_{air}$	total regional emission to air (annual average)	$[kg_c.d^{-1}]$	O
$Ereg_{ind}$	total regional emission to industrial soil (annual average)	$[kg_c.d^{-1}]$	O
$Ereg_{water}$	total regional emission to wastewater (annual average)	$[kg_c.d^{-1}]$	O
$Ereg_{direct\text{-}water}$	direct regional emission to surface water (annual average)	$[kg_c.d^{-1}]$	O

III.3.5 Continental emission rates

On the continental scale, all emissions for each compartment are summed over the relevant stages of the life cycle and the various applications, as was done for the regional scale.

$$Econt_j = \sum_{i=1}^{5} RELEASEcont_{i,j} \qquad j \in \{air, ind\} \tag{39}$$

$$Econt_{water} = Fconnect_{stp} \cdot \sum_{i=1}^{5} RELEASEcont_{i,water} \tag{40}$$

$$Econt_{direct-water} = RELEASEcont_{i,surf} + (1 - Fconnect_{stp}) \cdot \sum_{i=1}^{5} RELEASEcont_{i,water} \tag{41}$$

Input			
RELEASEcont$_{i,j}$	continental release during life-cycle stage *i* to compartment *j*	[kg$_c$.d^{-1}]	O
Fconnect$_{stp}$	fraction connected to sewer systems	[-]	D
Output			
Econt$_{air}$	continental emission to air (annual average)	[kg$_c$.d^{-1}]	O
Econt$_{ind}$	continental emission to industrial soil (annual average)	[kg$_c$.d^{-1}]	O
Econt$_{water}$	continental emission to wastewater (annual average)	[kg$_c$.d^{-1}]	O
Econt$_{direct-water}$	direct continental emission to surface water (annual average)	[kg$_c$.d^{-1}]	O

III.3.6 Local emission rates: release estimation for biocides

III.3.6.1 Product-type1: Human hygiene biocidal products

The scenarios and calculations used in this version of EUSES 2.1.1 for human hygiene biocidal products have been taken from the following document:

- Supplement to the methodology for risk evaluation of biocides Environmental Emission Scenarios for biocides used as human hygiene biocidal products (Product type 1) (European Commission DG ENV / RIVM, 2004).

This document can be obtained from the ECB Biocides website.

III.3.6.1.1 Private use of human hygiene biocidal products

Model for calculating concentrations in the municipal STP and surface water of biocides used in products like deodorants, antiperspirants, anti-dandruff shampoos, skin antiseptics, antimicrobial soaps and products to combat acne. It is possible to perform the calculations on A) the annual tonnage of the substance in the EU or in the region (if known), and B) the average consumption per inhabitant or C) the average consumption per application. For the average consumptions the average amounts may be entered by <u>volume</u> or by <u>weight</u>. The content may be entered as weight per volume or as weight per weight. The scenarios based on average consumption should be carried out for every product in which the specific biocide is applied.

A) Annual tonnage

$$TONNAGEreg = Fprodvol_{reg} \cdot TONNAGE \tag{42}$$

$$Elocal_{water} = TONNAGEreg \cdot Fmainsource_4 \cdot F_{4,water} \cdot \frac{365}{Temission_4} \tag{43}$$

Input			
TONNAGE	relevant tonnage in EU for this application	$[kg.d^{-1}]$	S
TONNAGEreg	relevant tonnage in the region for this application	$[kg.d^{-1}]$	S/O
$Fprodvol_{reg}$	fraction for the region	[-]	D
$Fmainsource_4$	fraction of the main source (local STP)	[-]	D
$F_{4,water}$	fraction released to wastewater	[-]	D
$Temission_4$	number of emission days	[d]	D
Output			
$Elocal_{water}$	local emission to waste water during episode	$[kg_c.d^{-1}]$	O

Table III-39 Default settings for calculating concentrations in the STP and surface water of compounds used in human hygiene products, based on annual tonnage

Parameter	**Symbol**	**Unit**	**Value**
Fraction for the region	$Fprodvol_{reg}$	[-]	0.1
Fraction of the main source (local STP)	$Fmainsource_4$	[-]	0.002
Fraction released to wastewater	$F_{4,water}$	[-]	1
Number of emission days	$Temission_4$	[d]	365

B) Average consumption per inhabitant

B1) Consumption by volume and content by weight per volume

$$Elocal_{water} = Nlocal \cdot F_{4,water} \cdot Vform_{inh} \cdot Cform_{volume} \cdot Fpenetr \qquad (44)$$

B2) Consumption by volume and content by weight per weight

$$Elocal_{water} = Nlocal \cdot F_{4,water} \cdot Vform_{inh} \cdot RHOform \cdot Cform_{weight} \cdot Fpenetr \qquad (45)$$

B3) Consumption by weight and content by weight per weight

$$Elocal_{water} = Nlocal \cdot F_{4,water} \cdot Qform_{inh} / RHOform \cdot Cform_{volume} \cdot Fpenetr \qquad (46)$$

B4) Consumption by weight and content by weight per volume

$$Elocal_{water} = Nlocal \cdot F_{4,water} \cdot Qform_{inh} \cdot Cform_{weight} \cdot Fpenetr \qquad (47)$$

C) Average consumption per application

C1) Consumption by volume and content by weight per volume

$$Elocal_{water} = Nlocal \cdot Nappl \cdot Finh \cdot F_{4,water} \cdot Vform_{appl} \cdot Cform_{volume} \cdot Fpenetr \qquad (48)$$

C2) Consumption by volume and content by weight per weight

$$Elocal_{water} = Nlocal \cdot Nappl \cdot Finh \cdot F_{4,water} \cdot Vform_{appl} \cdot RHOform \cdot Cform_{weight} \cdot Fpenetr \qquad (49)$$

C3) Consumption by weight and content by weight per weight

$$Elocal_{water} = Nlocal \cdot Nappl \cdot Finh \cdot F_{4,water} \cdot Qform_{appl} / RHOform \cdot Cform_{volume} \cdot Fpenetr \qquad (50)$$

C4) Consumption by weight and content by weight per volume

$$Elocal_{water} = Nlocal \cdot Nappl \cdot Finh \cdot F_{4,water} \cdot Qform_{appl} \cdot Cform_{weight} \cdot Fpenetr \qquad (51)$$

Input			
Nlocal	number of inhabitants feeding one STP	[eq]	D
$F_{4,water}$	fraction released to wastewater	[-]	D
$Cform_{volume}$	active substance in product	$[kg_c.m^{-3}]$	S
$Cform_{weight}$	active substance in product	$[kg.kg^{-1}]$	S
-	type of product	[-]	P
$Vform_{inh}$	consumption per inhabitant	$[l.d^{-1}]$	O
$Qform_{inh}$	consumption per inhabitant	$[kg.d^{-1}]$	O
$Vform_{appl}$	consumption per application	[l]	O
$Qform_{appl}$	consumption per application	[kg]	O
Nappl	number of applications per day	$[d^{-1}]$	O
Finh	fraction of inhabitants using the product	[-]	O
Fpenetr	penetration factor of disinfectant	[-]	D
RHOform	specific density of product	$[kg.m^{-3}]$	D
Output			
$Elocal_{water}$	local emission to waste water during episode	$[kg_c.d^{-1}]$	O

Table III-40 Default settings for calculating concentrations in the STP and surface water of compounds used in human hygiene products, based on average consumption

Parameter	**Symbol**	**Unit**	**Value**
Number of inhabitants feeding one STP	Nlocal	[eq]	10,000[a]
Fraction released to wastewater	$F_{4,water}$	[-]	1
Average consumption per inhabitant per day	$Vform_{inh}$ / $Qform_{inh}$	[$m^3.d^{-1}$] /[$kg.d^{-1}$]	
- anti-dandruff shampoo			-
- anti-perspirants/deodorants, aerosol			-
- anti-perspirants/deodorants, stick/roll-on			-
- creams			-
- mouth wash			-
Average consumption per application	$Vform_{appl}$ / $Qform_{appl}$	[$10^{-3}m^3$] /[kg]	
- anti-dandruff shampoo			0.0120[b]
- anti-perspirants/deodorants, aerosol			0.0030[b]
- anti-perspirants/deodorants, stick/roll-on			0.0005[b]
- creams			0.0008[e]
- mouth wash			0.0100
Number of applications per day	Nappl	[d^{-1}]	
- anti-dandruff shampoo			0.71[c]
- anti-perspirants/deodorants, aerosol			2.00[d]
- anti-perspirants/deodorants, stick/roll-on			1.00[b]
- creams			2.00[e]
- mouth wash			3.00
Fraction of inhabitants using the product	Finh	[-]	
- anti-dandruff shampoo			0.10
- anti-perspirants/deodorants, aerosol			0.20
- anti-perspirants/deodorants, stick/roll-on			0.80
- creams			0.10
- mouth wash			0.05
Penetration factor of disinfectant	Fpenetr	[-]	0.5
Specific density of product	RHOform	[$kg.m^{-3}$]	1,000

[a] already defined in the sewage treatment distribution sub module
[b] TGD (EC, 1996a)
[c] TGD: 2-7 times per week; default 5 times per week = 0.71 times per day
[d] TGD: 1-3 times per day
[e] Data from the TGD for facial cream: 1-2 times per day

III.3.6.1.2 Industrial use of human hygiene biocidal products

This model is used for calculating the concentrations in the municipal STP and surface water of biocides used in products like skin antiseptics, antimicrobial soaps and products for health care personnel hand wash. It is possible to perform the calculations on A) the annual tonnage of the substance in the EU or in the region (if known), and B) the average consumption per inhabitant or C) the average consumption per application. For the average consumptions the average amounts may be entered by volume or by weight. The content may be entered as weight per volume or as weight per weight.

A) Annual tonnage

$$TONNAGEreg = Fprodvol_{reg} \cdot TONNAGE \tag{52}$$

$$Elocal_{water} = TONNAGEreg \cdot Fmainsource_3 \cdot F_{3,water} \cdot \frac{365}{Temission_3} \tag{53}$$

Input

TONNAGE	relevant tonnage in EU for this application	$[kg.d^{-1}]$	S
TONNAGEreg	relevant tonnage in the region for this application	$[kg.d^{-1}]$	S/O
$Fprodvol_{reg}$	fraction for the region	[-]	D
$Fmainsource_3$	fraction of the main source (local STP)	[-]	D
$F_{3,water}$	fraction released to wastewater	[-]	D
$Temission_3$	number of emission days	[d]	D

Output

$Elocal_{water}$	local emission to waste water during episode	$[kg_c.d^{-1}]$	O

Table III-41 Default settings for calculating concentrations in the STP and surface water of compounds used in industrial use of human hygiene products, based on annual tonnage

Parameter	**Symbol**	**Unit**	**Value**
Fraction for the region	$Fprodvol_{reg}$	[-]	0.1
Fraction of the main source (local STP)	$Fmainsource_3$	[-]	0.007
Fraction released to wastewater	$F_{3,water}$	[-]	1
Number of emission days	$Temission_3$	[d]	365

B) Average consumption per bed

$$Elocal_{water} = Nbeds_{pres} \cdot Qsubst_{pres\_bed} \cdot F_{3,water} \tag{54}$$

$$Elocal_{water} = Nbeds_{occup} / Foccup \cdot Qsubst_{pres\_bed} \cdot F_{3,water} \tag{55}$$

C) Consumption per application

$$Elocal_{water} = Nbeds_{pres} \cdot Foccup \cdot Qsubst_{occup\_bed} \cdot F_{3,water} \tag{56}$$

$$Elocal_{water} = Nbeds_{occup} \cdot Qsubst_{occup\_bed} \cdot F_{3,water} \qquad (57)$$

Input

$Nbeds_{pres}$	number of beds in model hospital	[-]	D
Foccup	occupancy rate	[-]	D
$Nbeds_{occup}$	number of occupied beds in model hospital	[-]	D
$F_{3,water}$	fraction released to wastewater	[-]	D
-	specification of type of active ingredient used	[-]	P
$Qsubst_{pres\_bed}$	consumption of active ingredient per bed	[kg.d^{-1}]	O
-	specification of type of active ingredient used	[-]	P
$Qsubst_{occup\_bed}$	consumption of active ingredient per occupied bed	[kg.d^{-1}]	O

Output

$Elocal_{water}$	local emission to waste water during episode	[kg$_c$.d^{-1}]	O

Table III-42 Default settings for calculating concentrations in the STP and surface water of compounds used in industrial use of human hygiene products, based on average consumption

Parameter	**Symbol**	**Unit**	**Value**
Number of beds in model hospital	$Nbeds_{pres}$	[-]	400
Occupancy rate	Foccup	[-]	0.75
Number of occupied beds in hospital	$Nbeds_{occup}$	[-]	300
Average consumption of active ingredient per bed	$Qsubst_{pres\_bed}$	[kg.d^{-1}]	
- alcohols			1.5.10^{-2}
- quaternary ammonium compounds			4.0. 10^{-6}
- guanides			1.5. 10^{-5}
- compounds splitting off oxygen			3.8. 10^{-5}
- compounds splitting off halogen			1.0. 10^{-4}
- others			3.8. 10^{-5}
Consumption of active ingredient per occupied bed	$Qsubst_{occup\_bed}$	[kg.d^{-1}]	
- alcohols			2.0.10^{-2}
- quaternary ammonium compounds			5.0. 10^{-6}
- guanides			2.0. 10^{-5}
- compounds splitting off oxygen			5.0. 10^{-5}
- compounds splitting off halogen			1.3. 10^{-4}
- others			5.0. 10^{-5}
Fraction released to waste water	$F_{3,water}$	[-]	1

III.3.6.2 Product-type 2: Private area and public health area disinfectants and other biocidal products

The scenarios and models and calculation formulations used in this version of EUSES 2.1.1 for private area and public health area disinfectants and other biocidal products have been taken from the following document:

- EC (2003) and EC (2004)

This document can be obtained from the ECB Biocides website.

III.3.6.2.1 Sanitary sector

Private use of sanitary disinfectants

This scenario describes the private use of disinfectants for sanitary purposes. Releases take place to an STP, therefore, the STP is viewed as the local main source. The default fraction of 0.002 reflects the fraction of the total wastewater in the region, received by a large STP. In EUSES the standard STP is fed by 10,000 inhabitants with an amount of 0.2 m^3 per day. The emission calculations can be based on A) the annual tonnage or on B) the average consumption per capita.

A) Annual tonnage:

$$TONNAGEreg = Fprodvol_{reg} \cdot TONNAGE \qquad (58)$$

$$Elocal_{4,water} = TONNAGEreg \cdot Fmainsource_4 \cdot F_{4,water} \cdot \frac{365}{Temission_4} \qquad (59)$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_4$	[d]	365

Input

TONNAGE	quantity of a.i. used in the European Union	$[kg_c.d^{-1}]$	S
TONNAGEreg	quantity of a.i. used in the Netherlands	$[kg_c.d^{-1}]$	O/S
$Fprodvol_{reg}$	fraction for the region	[-]	D
$Fmainsource_4$	fraction of the local main source	[-]	D
$F_{4.water}$	Fraction released to waste water	[-]	D
$Temission_4$	number of emission days for sanitary proposes at private use	[d]	D
Output			
$Elocal_{4,water}$	local emission to wastewater	$[kg_c.d^{-1}]$	O
Temission	number of emission days	[d]	O

Table III-43 *Default settings for disinfectants for sanitary purposes at private use.*

Parameter	**Symbol**	**Unit**	**Value**
Fraction for the region	$Fprodvol_{reg}$	[-]	0.1
Fraction of the local main source for disinfectant	$Fmainsource_4$	[-]	0.002
Fraction released to waste water	$F_{4,water}$	[-]	1

B) average consumption per capita:

$$Elocal_{4,water} = Nlocal \cdot Vfrom \cdot Cform \cdot Fpenetr \cdot F_{4,water} \qquad (60)$$

Input

Nlocal	Number of inhabitants feeding one STP	[-]	D
$F_{4,water}$	Fraction released to waste water	[-]	D
Cform	concentration active substance in biocidal product	$[kg.m^{-3}]$	S
Fpenetr	Penetration factor of disinfectant	[-]	D
-	type of application	[-]	P
Vform	Consumption per capita	$[m^3.cap^{-1}.d^{-1}]$	O

Output

$Elocal_{4,water}$	Emission rate to waste water	$[kg.d^{-1}]$	O

Table III-44 *Default settings for calculating concentrations in the STP and surface water of compounds used in human hygiene products*

Parameter	**Symbol**	**Unit**	**Value**
Number of inhabitants feeding one STP	Nlocal	[-]	10,000[a]
Fraction released to waste water	$F_{4,water}$	[-]	1
Penetration factor of disinfectant	Fpenetr	[-]	0.5
Consumption per capita - general purpose (tiles floors, sinks) - lavatory	Vform	$[m^3.cap^{-1}.d^{-1}]$	 5.10^{-6} 2.10^{-6}

[a] already defined in the sewage treatment distribution sub module

III.3.6.2.2 Medical sector

Professional use

Disinfection of rooms, furniture and objects

Two models are used to calculate the release of disinfectants used for sanitary purposes in hospitals, viz. based on A) the annual tonnage and B) based on the applied amount of aqueous solution.

A) Annual tonnage:

$$TONNAGEreg = Fprodvol_{reg} \cdot TONNAGE \tag{61}$$

$$Elocal_{3,water} = TONNAGEreg \cdot Fhospital \cdot F_{3,water} \cdot \frac{365}{Temission_{3}} \tag{62}$$

Input			
TONNAGE	relevant tonnage in EU for this application	[kg.d^{-1}]	S
TONNAGEreg	relevant tonnage in the region for this application	[kg.d^{-1}]	S
$Fprodvol_{reg}$	fraction for the region	[-]	D
Fhospital	fraction for the hospital	[-]	D
$F_{3,water}$	fraction released to wastewater	[-]	D
$Temission_3$	number of emission days	[d]	D
Output			
$Elocal_{3,water}$	local emission to waste water during episode	[kg$_c$.d^{-1}]	O

Table III-45 *Default settings for calculating concentrations in the STP and surface water of compounds used in disinfection of rooms, furniture and objects based on the annual tonnage*

Parameter	Symbol	Unit	Value
Fraction for the region	$Fprodvol_{reg}$	[-]	0.1
Fraction for the hospital	Fhospital	[-]	0.007
Fraction released to wastewater	$F_{3,water}$	[-]	0.75
Number of emission days	$Temission_3$	[d]	260

B) Amount of solution used:

Sanitary purposes

$$Elocal_{3,water} = Vcons_{san} \cdot Cproc_{san} \cdot Fsan \tag{63}$$

Brushes

$$Elocal_{3,water} = Vcons_{obj} \cdot Cproc_{obj} \cdot Fobj \tag{64}$$

Sanitary purposes and brushes

$$Elocal_{3,water} = Vcons_{san} \cdot Cproc_{san} \cdot Fsan + Vcons_{obj} \cdot Cproc_{obj} \cdot Fobj \tag{65}$$

Input			
Fsan	fraction released to waste water for sanitary purposes	[-]	D
Fobj	fraction released to waste water for brushes	[-]	D
$Cproc_{san}$	concentration at which active substance is used, sanitary purposes	[$kg.m^{-3}$]	S
$Cproc_{obj}$	concentration at which active substance is used, brushes	[$kg.m^{-3}$]	S
$Vcons_{san}$	amount of water with active substance, sanitary purpose	[$m^3.d^{-1}$]	D
$Vcons_{obj}$	amount of water with active substance, brushes	[m^3d^{-1}]	D
Output			
$Elocal_{3,water}$	emission rate to waste water	[$kg.d^{-1}$]	O

Table III-46 *Default settings for calculating concentrations in the STP and surface water of compounds used in disinfection of room, furniture and objects based on the amount of solution used on a day*

Parameter	**Symbol**	**Unit**	**Value**
Fractions release to waste water			
- sanitary purposes	Fsan	[-]	0.55
- brushes	Fobj	[-]	0.95
Amount of water with active substance			
- sanitary purposes	$Vcons_{san}$	[m^3]	0.025
- brushes	$Vcons_{obj}$	[m^3]	0.025

Above a certain tonnage the scenario based on the tonnage should be applied preferably. If the default values are filled out in the formulas for the calculation of the local emissions to wastewater, $Elocal_{water}$, the break-even point can be written in the form:

$$\boldsymbol{TONNAGEreg = 956 \cdot Cproc_{san}} \qquad \text{sanitary purposes}$$

$$\boldsymbol{TONNAGEreg = 1560 \cdot Cproc_{obj}} \qquad \text{brushes}$$

$$\boldsymbol{TONNAGEreg = 956 \cdot Cproc_{san} + 1560 \cdot Cproc_{obj}} \qquad \text{sanitary purposes and brushes}$$

Disinfection of instruments

There are two types of washers: a) washers/disinfectors with replacement of the disinfectant solutions at regular intervals (called "replacement" in the scenario) and b) washers/disinfectors where a fresh disinfectant solution is applied every disinfection operation; the substance is discarded into the sewer after disinfection (called "once-through" in the scenario). Other instruments are disinfected in solutions (or suspensions) of disinfectants to prevent adhesion of blood, pus, etc. These baths are discarded into the sewer after use. If a biocide is notified for both disinfection of scopes and other instruments, the emission for a single point source (one hospital) should be calculated by summing the results of both emission scenarios. It is assumed that in case of more than one washers or disinfectors replacement of all machines occurs on the same day.

Washers or disinfectors, replacement:

Concentration at day of replacement due to carry-over

$$Cproc_{carry\_over} = \frac{Cproc}{(1 + Fcarry\_over)^{Tint_{repl}}} \qquad (66)$$

Concentration at day of replacement including conversion

$$Cproc_{repl} = Cproc_{carry\_over} \cdot e^{-kdeg_{disinf} \cdot Tint_{repl}} \qquad (67)$$

$$Elocal_{3,water} = Nmax_{mach} \cdot Vproc \cdot Cproc_{repl} \qquad (68)$$

Washers or disinfector, once through

$$Elocal_{3,water} = Nmax_{mach} \cdot Vproc \cdot Cproc \qquad (69)$$

Input			
Cproc	working concentration of active ingredient	[kg.m^{-3}]	S
Nmax$_{mach}$	number of washers or disinfectors	[-]	D
-	type of washer	[-]	P
Vproc	volume of solution in machine	[m^3]	O
Tint$_{repl}$	Replacement interval	[d]	D
Fcarry_over	Fraction carry-over	[-]	D
kdeg$_{disinf}$	Rate constant for chemical conversion	[d^{-1}]	S/D
Output			
Elocal$_{3,water}$	emission rate to waste water	[kg.d^{-1}]	O

Table III-47 *Default settings for calculating concentrations in the STP and surface water of compounds used in disinfection of instruments with washers or disinfectors*

Parameter	Symbol	Unit	Value
Maximum number of washers or disinfectors	Nmax$_{mach}$	[-]	3
Volume of solution in machine - replacement - once through	Vproc	[m^3]	 0.1 0.01
Replacement interval (replacement)	Tint$_{repl}$	[d]	14
Fraction carry-over (replacement)	Fcarry-over	[-]	0.015
Rate constant for chemical conversion (replacement)	kdeg$_{disinf}$	[d^{-1}]	0

Disinfection of instruments in baths:

$$Tint_{repl} = INT(1/Temission_3 + 0.5) \qquad (70)$$

$$Elocal_{3,water} = \frac{Qsubst}{Temission_3} \cdot e^{-kdeg_{disinf} \cdot Tint_{repl}} \qquad (71)$$

Input

$Tint_{repl}$	average time disinfection solution is in use (replacement interval)	[d]	O
Qsubst	amount of active substance used	[$kg.d^{-1}$]	D
$Temission_3$	emission day, i.e., replacements	[d^{-1}]	D
$kdeg_{disinf}$	rate constant for chemical conversion	[d^{-1}]	S/D

Output

$Elocal_{3,water}$	emission rate to waste water	[$kg.d^{-1}$]	O

Table III-48 *Default settings for calculating concentrations in the STP and surface water of compounds used in disinfection of instruments with washers or disinfectors*

Parameter	**Symbol**	**Unit**	**Value**
Amount of active substance used	Qsubst	[$kg.d^{-1}$]	0.68
Emission day, i.e., number of replacements	$Temission_3$	[d^{-1}]	0.27
Rate constant for chemical conversion (replacement)	$kdeg_{disinf}$	[d^{-1}]	0

Laundry disinfectants

Two emission scenarios are presented, one for commercial laundries where hospitals send their laundry and one for laundries or hospitals using tumbler washing machines. The size of commercial laundries can vary considerably but large laundries may have three or more washing tubes with a capacity of 8000 kg.day-1 per tube, producing 48 $m^3.day^{-1}$ of waste. It is assumed here that a commercial laundry connected to the standard STP of EUSES/USES (2000 m^3 waste water per day) can have three washing tubes (3 * 48 = 144 m^3 wastewater per day). On the other hand, the situation is considered where a hospital is doing its own laundry or where the contaminated laundry is done at a commercial laundry using a tumbler washing machine. It is estimated that per kg of dirty laundry 6 g of detergent ("soap") is used, 4 g for soaking and 2 g for the washing cycle. In the case of disinfection, it is estimated that about 10% of the amount of soap are disinfectant.

Washing streets

$$Elocal_{3,water} = Nmach \cdot Qmat \cdot Vform_{kg} \cdot Cform \cdot (1 - Fred) \qquad (72)$$

Input

Nmach	number of washing tubes (with disinfectant)	[-]	D
Qmat	capacity of washing tube	[$kg.d^{-1}$]	D
$Vform_{kg}$	amount of disinfectant for laundry	[$m^3.kg^{-1}$]	S
Cform	concentration of active substance in disinfectant solution	[$kg.m^{-3}$]	S
Fred	concentration reduction in washing process	[-]	D

Output

$Elocal_{3,water}$	emission rate to waste water	[$kg.d^{-1}$]	O

Table III-49 *Default settings for calculating concentrations in the STP and surface water of disinfectants used for doing biologically contaminated laundry from hospitals in washing streets*

Parameter	**Symbol**	**Unit**	**Value**
Number of washing tube	Nmach	[-]	3
Capacity of washing tube	Qmat	[kg.d^{-1}]	8,000
Concentration reduction in washing process	Fred	[-]	0

Washing machines

$$Elocal_{3,water} = Nbatch \cdot Qmat \cdot Vform_{kg} \cdot Cform \cdot (1 - Fred) \qquad (73)$$

Input

Nbatch	number of batches	[-]	D
Qmat	capacity of machines	[kg]	D
$Vform_{kg}$	amount of disinfectant for laundry	[m^3.kg^{-1}]	S
Cform	concentration of active substance in disinfectant solution	[kg.m^{-3}]	S
Fred	concentration reduction in washing process	[-]	D
Output			
$Elocal_{3,water}$	emission rate to waste water	[kg.d^{-1}]	O

Table III-50 *Default settings for calculating concentrations in the STP and surface water of disinfectants used for doing biologically contaminated laundry from hospitals in tumbler washing machines*

Parameter	**Symbol**	**Unit**	**Value**
Number of washing tubes	Nmach	[-]	3
Capacity of washing tube	Qmat	[kg.d^{-1}]	8,000
Concentration reduction in washing process	Fred	[-]	0

III.3.6.3 Product type 5: Drinking water disinfectants

The scenarios and models and calculation formulations used in this version of EUSES 2.1.1 for drinking water disinfectants have been taken from the following document:

- Emission scenario document on Drinking water desinfectants (Herrmann & Wagner, 2003).

This document can be obtained from the ECB Biocides website.

In addition to this document it is decided to set a default emission equal to 365 days.

III.3.6.3.1 Drinking water disinfectants

The model calculates the concentration of drinking water disinfectants in the influent of the sewage treatment plant (STP) based on concentrations of the disinfectants in drinking water when leaving the tap. Degradation in the residence time in the sewer system is also taken into account.

$$Clocal_{inf} = C_{drinkingwater} \cdot e^{-kdeg \cdot Tsewer} \qquad \textbf{(74)}$$

Input

$C_{drinkingwater}$	maximum concentration in drinking water at the tap	$[mg_c.l^{-1}]$	S
kdeg	degradation rate constant in the sewer system	$[d^{-1}]$	S
T_{sewer}	residence time in the sewer system	[d]	D

Output

$Clocal_{inf}$	concentration in untreated wastewater	$[mg_c.l^{-1}]$	O

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_{drink}$	[d]	365

Table III-51 Default settings for calculating concentrations in the STP and surface water of drinking water disinfectants

Parameter	**Symbol**	**Unit**	**Value**
Maximum concentration in drinking water	$C_{drinkingwater}$	$[mg.l^{-1}]$	-
Degradation rate constant in sewer system	kdeg	$[d^{-1}]$	[-]
Residence time in the sewer system	T_{sewer}	[d]	0.042

III.3.6.4 Product type 6: In-can preservatives

The scenarios and models and calculatios used in this version of EUSES 2.1.1 for in-can preservatives have been taken from the following documents:

- Washing and cleaning fluids: van der Poel and Bakker (2002) and RIVM, VROM and VWS (2002).

This document can be obtained from the ECB Biocides website.

For all the scenarios, except washing and cleaning fluids the release from professional industrial and private use is already covered by other product types. In order to determine the emission and environmental concentrations the EUSES 2.1.1 program makes reference to the product types to be selected. For washing and cleaning fluids, the release from, professional and private use is presented.

III.3.6.4.1 Washing and cleaning fluids

The same emission scenario as for product type 1, human hygiene biocidal products can be used, see section III.3.6.1. Private use of human hygiene biocidal products. Only specific tables with consumption data have been introduced for this scenario.

Table III-52 Pick-list for average consumptions per inhabitant per day, $Vform_{inh}$ $[10^{-3}m^3.d^{-1}]$ &$Qform_{inh}$ $[kg.d^{-1}]$, per application, $Vform_{appl}$ $[.10^{-3}m^3]$ & $Qform_{appl}$ [kg], number of applications, Nappl $[d^{-1}]$, and the fraction of inhabitants using the product, Finh [-].

Product	**$Vform_{inh}$** **$Qform_{inh}$**	**$Vform_{appl}$** **$Qform_{appl}$**	**Nappl**	**Finh**
Fabric washing				
- washing liquids	0.004			
- auxiliary products	0.0006			
- fabric rinsing products	0.007			
Washing-up liquid				
- hand wash	0.007			
- machine wash	0.0016			
Cosmetics				
- hair conditioner (cream rinse)		0.014	0.2	0.3
- hair conditioner		0.0027	0.75	0.3
- hair gel		0.0029	1	0.2
Permanent wash fluid				
- curling fluid		0.08	0.01	0.1
- fixing fluid		0.0	0.01	0.1
- eye shadow		0.00001	2	0.3

- mascara		0.000025	1	0.2
- eye liner		0.000005	1	0.1
- lipstick, lip ointment		0.0001	4	0.3
Human hygiene products				
- toilet soaps	0.0016			
-shampoo	0.0023			
-shower products		0.005	0.9	0.95
-bath products		0.017	0.2	0.15
Anti-perspirants/deodorants				
- aerosol		0.003	2	0.2
- stick, roll-on		0.0005	1	0.8
Creams				
- general creams		0.001	1.5	0.2
- facial creams		0.0008	2	0.1
- body lotion		0.0075	1.5	0.2
- hand cream		0.0003	2	0.5
Suntan products				
- creams		0.008	2	0.4
- lotions		0.010	2	0.4

III.3.6.4.2 Fluids used in paper production

See product type 7 section III.3.6.11, Preservatives used in paper production.

III.3.6.4.3 Textile processing industry

See Product type 9, section III.3.6.33, Textile processing industry using textile preservatives.

III.3.6.4.4 Leather industry

See section III.3.6.32, Leather preservatives from product type 9

III.3.6.5 Product type 7: Film preservatives

The scenarios and models and calculation formulations used in this version of EUSES 2.1.1 for film preservatives have been taken from the following documents:

- Paints and coatings: supplement to the methodology for risk evaluation of biocides Environmental Emission Scenarios for biocides used as Film Preservatives (Product type 7) (European Commission DG ENV / RIVM, 2004)
- Pulp, paper and board industy (EC, 2004).

This document can be obtained from the ECB Biocides website.

III.3.6.5.1 Pulp, paper and board industry

The emission scenario document comprises life cycle stages 3 (industrial use) and 6 (waste). For life cycle stage 3 the emission scenario calculates air releases from the drying sections after size-pressing and releases to wastewater from "broke" in the paper machine at stock preparation. For life cycle stage 6 the emission scenario calculates releases to wastewater resulting from paper recycling. The scenarios presented in this section are the same for in-can preservatives (PT 6) and fibre preservatives (PT 9).

Life cycle stage Industrial use

Releases from drying sections after size-pressing and coating

$$P_{T2} = P_{T1} \cdot e^{\frac{\Delta H}{R}\left(\frac{1}{T_1} - \frac{1}{T_2}\right)} \tag{75}$$

$$Qsubst = Vform \cdot Cform \tag{76}$$

$$Elocal_{3,air} = Qpaper \cdot Qsubst \cdot Fevap \cdot (1 - Fdecomp) \tag{77}$$

Input			
Vform	volume of product with preservative applied per kg of paper	$[m^3.kg^{-1}]$	S
Cform	concentration of active substance in the biocidal product	$[kg_c.m^{-3}]$	S
Qsubst	quantity of active substance applied per kg of paper	$[kg_c.kg^{-1}]$	S/O
-	type of paper produced	[-]	P
Qpaper	quantity of coated paper produced per day	$[kg.d^{-1}]$	O
P_{T1}	vapour pressure at standard temperature	[Pa]	S
P_{T2}	vapour pressure at relevant application temperature	[Pa]	O
ΔH	heat of vaporisation for relevant temperature range	$[kJ.mol^{-1}]$	S
R	universal gas constant	$[kJ.mol^{-1}.K^{-1}]$	D
T_1	standard temperature at which P_{T1} is measured	[K]	S
T_2	relevant application temperature	[K]	S
Fevap	fraction evaporated	[-]	O
Output			
$Elocal_{3,air}$	local emission of active substance to air	$[kg_c.d^{-1}]$	O

Table III-53 *Defaults for emission calculations.*

Parameter	**Symbol**	**Unit**	**Value**
vapour pressure at standard temperature	P_{T1}	[Pa]	1)
heat of vaporisation	ΔH	[kJ.mol^{-1}]	1)
universal gas constant	R	[kJ.mol^{-1}.K^{-1}]	8.314
standard temperature at which P_{T1} is measured	T_1	[K]	298 2)
relevant application temperature	T_2	[K]	373

1) substance specific properties

2) when no standard temperature is given a default value of 25 °C is used

Table III-54 *Default settings for calculating release to air of biocidal compounds used as in-can preservatives from the drying sections after size-pressing and coating in paper production*

Parameter	**Symbol**	**Unit**	**Value**
Quantity of coated paper produced per day	Qpaper	[kg.d^{1}]	
- news print			449,000
- printing and writing paper			66,000
- printing and cardboard for packaging			237,000
- paper for sanitary and domestic use (tissue paper)			222,000
- special and industrial paper (all types)			102,000
Cardboard			
- flat cardboard			329,000
- corrugated cardboard			329,000
Fraction evaporated if volatility (Pa at 100 °C)	Fevap	[-]	
≥ 133			0.0025
13.3-133			0.0005
1.3-13.3			0.0001
<1.3			0
Fixation fraction	Ffix	[-]	
PT 6			0
PT 7			0.8
PT 9			0.8
Fraction decomposed during drying	Fdecomp	[-]	0

Releases from “broke”

$$Qsubst = Vform \cdot Cform \tag{78}$$

$$Elocal_{3,water} = Qpaper \cdot Qsubst \cdot Fbroke \cdot (1 - Ffix) \cdot (1 - Fclosure) \tag{79}$$

Input			
Vform	volume of product with preservative applied per kg of paper	[$m^3.kg^{-1}$]	S
Cform	concentration of active substance in the biocidal product	[$kg_c.m^{-3}$]	S
Qsubst	quantity of active substance applied per kg of paper	[$kg_c.kg^{-1}$]	S/O
-	type of paper produced	[-]	P
Qpaper	quantity of coated paper produced per day	[$kg.d^{-1}$]	O
Fbroke	fraction of coated broke produced compared to overall production	[-]	D
Ffix	fixation fraction	[-]	D
Fclosure	degree of closure of the water system	[-]	O
Output			
$Elocal_{3,water}$	local emission of active substance to waste water	[$kg_c.d^{-1}$]	O

***Table III-55** Default settings for calculating release to waste water of biocidal compounds used as in-can preservatives from “broke” in paper production*

Parameter	Symbol	Unit	Value
Degree of closure of the water system¹⁾	Fclosure	[-]	
- news print			0.75²⁾
- printing and writing paper			0.55³⁾
- printing and cardboard for packaging			0.80⁴⁾
- paper for sanitary and domestic use (tissue paper)			0.75²⁾
- special and industrial paper (all types)			0.55³⁾
Cardboard			
- flat cardboard			0.80⁴⁾
- corrugated cardboard			0.80⁴⁾
Fraction of coated broke produced compared to overall production	Fbroke	[-]	0.2
Fixation fraction	Ffix	[-]	0

1) the degree of closure will not effect the concentration of a substance in the wastewater, it will determine the volume of water and therefore the total amount of substance emitted. The wastewater flow should be adjusted accordingly when the degree of closure is changed.

2) a range of 0.65-0.85 was given in the ESD, 0.75 has been chosen as the average value

3) a range of 0.4-0.7 was given in the ESD, 0.55 has been chosen as the average value

4) a range of 0.65-0.95 and above was given in the ESD, 0.80 has been chosen as the average value

Life cycle stage waste treatment

Paper recycling

$$TONNAGEreg = Fprodvol_{reg} \cdot TONNAGE \qquad (80)$$

$$Elocal_{6,water} = TONNAGEreg \cdot Frec \cdot Fmainsource_{5} \cdot Fdeink \cdot \left(1 - Fprelim\right) \cdot \left(1 - Fdecomp\right) \cdot \frac{365}{Nwdays} \qquad (81)$$

Input			
TONNAGE	relevant tonnage in EU for this application	$[kg.d^{-1}]$	S
TONNAGEreg	relevant tonnage in the region for this application	$[kg.d^{-1}]$	S/O
$Fprodvol_{reg}$	fraction for the region	[-]	D
$Fmainsource_{6}$	fraction of the main source (local STP)	[-]	D
-	type of paper recycled	[-]	P
Frec	fraction of paper recycled	[-]	O
Fdeink	fraction of preservatives released at de-inking	[-]	D
Fdecomp	fraction decomposed during de-inking	[-]	D
-	degree of solubility	[-]	P
Fprelim	fraction removed from waste water during preliminary on-site treatment	[-]	O
Nwdays	number of working days	[d]	D
Output			
$Elocal_{6,water}$	local emission of active substance to waste water	$[kg_{c}.d^{-1}]$	O

Table III-56 *Default settings for calculating releases of in-can preservatives from paper recycling*

Parameter	**Symbol**	**Unit**	**Value**
Fraction for the region	$Fprovol_{reg}$	[-]	0.1
Fraction of the main source	$Fmainsource_{6}$	[-]	0.1
Fraction of recycled paper - news print - printing and writing paper - paper and cardboard for packaging - paper for sanitary and domestic use (tissue paper) - special and industrial paper (all types) Cardboard - flat cardboard - corrugated cardboard	Frec	[-]	0.54 0.58 0.11 0.46 0.54 0.55 0.92 0.90
Fraction of preservatives released at de-inking	Fdeink	[-]	1
Fraction decomposed during de-inking	Fdecomp	[-]	0
Fraction removed from wastewater during preliminary on-site treatment	Fprelim	[-]	

Parameter	Symbol	Unit	Value
- easy soluble[1] - poorly soluble			0.1 0.7
Number of working days	Nwdays	[d]	340

[1] Easy soluble substances are defined as having a water solubility >1000 mg.l^{-1}. A range of 0-0.2 has been given in the ESD for easy soluble substance and a range of 0.5-0.9 has been reported for poorly soluble substances.

III.3.6.5.2 Paints and coatings

Formulation

For emissions of biocides used as film preservatives the default A- and B-tables or the emission scenario document (ESD) from the TGD (2003) can be used for IC 14 Paints, lacquers and varnished industry, see also product type 6 section III.3.6.7, Paints and coatings.

Private and proffesional use, sevice life and waste

Film preservatives are only present in decorative paints, which are used by the public at large or professional painters. Thus paint application may be carried out by public at large and professionals at a relatively small scale. Paints may be applied, for example, by brush, rollers or spraying and will vary depending on the way of application and. As paint application is not a typical biocide application no emission scenarios have been developed specifically. For emission estimation the scenarios for new and existing substances may be applied. In the EA-UK document (EA-UK, 2002) an emission scenario document is found for industrial category 14 (Paints, lacquers and varnishes industry). Emission factors for decorative paint types are presented for the use of coatings (private and professional use) and also covers disposal of the coated product or removed paint (waste stage). The emission factors presented refer only to solids. Emissions are determined analogous to the stage of formulation as are the fraction of the main source and number of emission days. The calculations present the emission on the regional scale as a fraction of the regional tonnage. The local scale can be modelled starting from the sewage treatment plant (STP). Regional emissions are calculated for as wel water, soil and waste in the original ESD. For the exposure to biocides the emissions on the regional scale seem not to be the most relevant though. For this reason the regional release is no considered in EUSES 2.1. Furthermore, the relase to waste is not a standard compartment in EUSES.

$$TONNAGE = F_{a.i.} \cdot TONNAGEpaint \qquad (82)$$

$$TONNAGEreg = Fprodvol_{reg} \cdot TONNAGE \qquad (83)$$

$$Elocal_{water} = TONNAGEreg \cdot Fmainsource_{3} \cdot F_{3,water} \cdot \frac{365}{Temission_{3}} \qquad (84)$$

Input			
TONNAGEpaint	tonnage of paint used in the EU containing the preservative	$[kg.d^{-1}]$	S
$F_{a.i.}$	Fraction of the film preservative in the product	[-]	D
TONNAGE	relevant tonnage in EU for this application	$[kg.d^{-1}]$	S
TONNAGEreg	relevant tonnage in the region for this application	$[kg.d^{-1}]$	S/O
$Fprodvol_{reg}$	fraction for the region	[-]	D
$Fmainsource_3$	fraction of the main source	[-]	O
$Temission_3$	number of emission days	[d]	O
$F_{3,water}$	fraction released to wastewater during application	[-]	D
$F_{3,waste}$	fraction released to waste during application	[-]	D
$F_{4,soil}$	fraction released to soil during service life	[-]	D
$F_{5,waste}$	fraction released to waste during removal	[-]	D
Output			
$Elocal_{water}$	local emission to water	$[kg_c.d^{-1}]$	O

Table III-57 Default settings for calculating concentrations of film preservatives used in coating products

Parameter	**Symbol**	**Unit**	**Value**
Fraction of the film preservative in the paint	$F_{a.i.}$	[-]	0.01
Fraction for the region	$Fprodvol_{reg}$	[-]	0.1

Table III-58 Emission factors to air $F_{3,air}$ and (waste)water $F_{3,water}$ for the application of decorative paint and coating products that are likely to contain film preservatives.

Parameter	**Symbol**	**Unit**	**Value**	
			private	**professional**
Fraction released to water during application	$F_{3,water}$	[-]	0.03	0
Fraction disposed of as waste during application	$F_{3,waste}$	[-]	0.25	0.07
Fraction to soil from paint during service life	$F_{4,soil}$	[-]	0.02	0.03
Fraction disposed of as waste at the end of life (waste stage)	$F_{5,waste}$	[-]	0.70	0.90

** assuming treatment of flue gasses (0.98 if no treatment)*

Table III-59 Fraction of the main source, $Fmainsource_3$ [-], and the number of emission days, $Temission_3$ [d], for the private and professional use of paints and coatings with in-can preservatives based on the corrected regional tonnage, $TONNAGEreg_{form}$ $[tonnes .yr^{-1}]$, of the biocide

$\mathbf{TONNAGEreg_{form}}$	$\mathbf{Fmainsource_3}$	$\mathbf{Temission_3}$
< 500	0.002	150
≥500	0.002	300

III.3.6.5.3 Polymers industry

See section III.3.6.36, Polymerised materials preservatives under product type 9.

III.3.6.6 Product type 8: Wood preservatives and wood protectors

The scenarios and models and calculation formulations used in this version of EUSES 2.1.1 for wood preservatives have been taken from the following document:

- OECD Series on Emission Scenario Documents. Number 2 Emission Scenario Document for Wood Preservatives Parts I to IV.

This document can be obtained from the ECB Biocides website and from the OECD.

Since the ESD was first published discussions have taken place on a number of the parameters and the default values that have been included in the models.A number of recommendations for changing the default values have taken been made at Biocides Technical Meetings and then confirmed at Biocides Competent Authority meetings.Users of the EUSES 2.1.1 in the evaluation of wood preservatives (PT08) for the purposes of the Biocidal Products Directive (98/8/EC) should be aware that the default values included in the version they are using may not contain the latest decisions which have been made. Efforts should be made to obtain these and the ECB Biocides / COM should be approached for the latest values and insert them in their programme. It is envisaged that a formal procedure and documentary record of the decisions made on default values will be established. It is recommended that the user separately records in a table any changes made to the current default values used in the calculations for their risk assessments

The following modifications have been made:
Equation for calculating the volume of the soil compartment have been added. Furthermore the default value for the soil depth and distance from the source have been set to 0.5 m instead of the original value of 0.1 m.

Industrial use

III.3.6.6.1 Scenario for wood preservation through automated spraying

Parameters/variables and default values for automated spraying.

Solid application rate: $Q_{a.i.} = Qform \cdot F_{a.i.}$ **(85)**

Fluid application rate $Q_{a.i.} = Vform \cdot RHOform.F_{a.i.}$ **(86)**

$$Elocal_{3,air} = Q_{a.i.} \cdot AREA_{wood-treated} \cdot \left(F_{3,air} + F_{drift}\right) \qquad \textbf{(87)}$$

$$Elocal_{3,water} = Q_{a.i.} \cdot AREA_{wood-treated} \cdot F_{3,water} \qquad \textbf{(88)}$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_3$	[d]	250
RIVERFLOW	$FLOW_{surfacewater}$	[$m^3.d^{-1}$]	25920

Input

$AREA_{wood\text{-}treated}$	area of wood treated per day	[$m^2.d^{-1}$]	D
VP	vapour pressure	[Pa]	S
SOL	water solubility	[$kg_c.m^{-3}$]	S
$F_{3,air}$	fraction released to air	[-]	O^c
$F_{3,water}$	fraction released to waste water	[-]	O^c
Qform	solid application rate of applied formulation	[$kg.m^{-2}$]	S
Vform	fluid application rate of applied formulation	[$m^3.m^{-2}$]	S
RHOproduct	density of product	[$kg.m^{-3}$]	S
$F_{a.i.}$	fraction of active ingredient in formulation	[-]	S
$Temission_3$	number of emission days for industrial use (including storage)	[d]	D

Output

$Q_{a.i.}$	quantity of active ingredient applied per m^2 of wood	[$kg.m^{-2}$]	S/O
$Elocal_{3,water}$	local emission to waste water	[$kg_c.d^{-1}$]	O
$Elocal_{3,air}$	local emission to air during episode	[$kg_c.d^{-1}$]	O

Table III-60 Default settings for automated spraying.

Parameter	**Symbol**	**Unit**	**Value**
Area of wood treated per day	$AREA_{wood\text{-}treated}$	[$m^2.d^{-1}$]	
small plants			2 000
large plants			20 000
Quantity of active ingredient applied per unit of wood-area	Q_{ai}	[$kg.m^{-2}$]	-
Fraction released to waste water *Solubility in water [mg.m^{-3}]*	$F_{3,water}$	[-]	
<0.25			0.0001
0.25 – 1			0.0015
1 – 50			0.003
50-100			0.015
≥ 100			0.03
Fraction released to air *Vapour pressure at 20 °C [Pa]*	$F_{3,air}$	[-]	
<0.005			0.001
0.005 - 0.05			0.01
0.05 - 0.5			0.02
0.5 - 1.25			0.075
1.25 - 2.5			0.15
≥2.5			0.25
Fraction of spray drift	F_{drift}	[-]	0.001

Parameters/variables and default values for storage at automated spraying facility.
In the EUSES 2.1.1 program the concentration of substance in surface water after emissionof process water via STP and due to run-off are presented separately. The concentration in surface water after emission of process water via an STP is presented in the sheet on locan concentration and depositions.

$$AREA_{storage} = \frac{Tstorage \cdot V_{wood-treated}}{D_{wood-stacked}} \tag{89}$$

$$Qsoil = AREA_{storage} \cdot DEPTHsoil \cdot RHOsoil \tag{90}$$

$$Elocal_{storage,soil} = FLUX_{storage} \cdot AREA_{wood-exposed} \cdot AREA_{storage} \cdot (1 - F_{runoff}) \tag{91}$$

$$Csoil_{ini} = \frac{Elocal_{storage,soil} \cdot Temission_{ini}}{Qsoil} \tag{92}$$

$$Csoil_{chron} = \frac{Elocal_{storage,soil} \cdot Temission_{chron}}{Qsoil} \tag{93}$$

$$Elocal_{storage,\ water} = FLUX_{storage} \cdot AREA_{wood-exposed} . AREA_{storage} \cdot F_{runoff} \tag{94}$$

$$Cwater_{run-off} = \frac{Elocal_{storage,water}}{FLOW_{surfacewater}} \tag{95}$$

$$Cwater_{processwater} = \frac{Clocal_{eff} \cdot EFFLUENTlocal_{stp}}{FLOW_{surfacewater}} \tag{96}$$

$$Cwater_{total} = \frac{Elocal_{storage,water}}{FLOW_{surfacewater}} + \frac{Clocal_{eff} \cdot EFFLUENTlocal_{stp}}{FLOW_{surfacewater}} \tag{97}$$

Input			
Tstorage	duration of storage of treated wood prior to shipment	[d]	D
$V_{\text{wood-treated}}$	volume of wood treated per day	$[m^3.d^{-1}]$	D
$D_{\text{wood-stacked}}$	storage density of treated wood stacked on storage area	$[m^3.m^{-2}]$	D
DEPTHsoil	depth of soil	[m]	D
RHOsoil	wet soil bulk density	$[kg_{wwt}.m^{-3}]$	O^c
$FLUX_{\text{storage}}$	average daily flux of the a.i during the storage period	$[kg_c.m^{-2}.d^{-1}]$	S
$AREA_{\text{wood-exposed}}$	effective surface area of treated wood exposed to rain per unit of storage area	$[m^2.m^{-2}]$	D
F_{runoff}	fraction of rainwater running off the storage site	[-]	D
$Elocal_{\text{stroage,soil}}$	local emission to soil from storage	$[kg_c.d^{-1}]$	O
$Temission_{\text{ini}}$	duration of the initial assessment period	[d]	D
$Temission_{\text{chron}}$	duration of the chronic assesssment period	[d]	S
$FLOW_{\text{surfacewater}}$	volume flow rate of creek/river	$[m^3.d^{-1}]$	D
$Clocal_{\text{eff}}$	sewage treatment plant effluent concentration (EUSES output)	$[kg_c.m^{-3}]$	O^c
$EFFLUENTlocal_{\text{stp}}$	effluent flow of the local sewage treatment plant	$[m^3.d^{-1}]$	O^c
$AREA_{\text{storage}}$	surface area of the storage place	$[m^2]$	D/O
Output			
Qsoil	wet soil mass	$[kg_{wwt}]$	O
$Elocal_{3,\text{air}}$	local emission to air	$[kg_c.d^{-1}]$	O
$Elocal_{3,\text{ water}}$	local emission to surface water	$[kg_c.d^{-1}]$	O
$Elocal_{\text{storage, water}}$	local emission to surface water from storage	$[kg_c.d^{-1}]$	O
$Csoil_{\text{ini}}$	concentration of substance in soil for initial assessment period	$[kg_c.kg^{-1}{}_{wwt}]$	O
$Csoil_{\text{chron}}$	concentration of substance in soil for longer assessment period	$[kg_c.kg^{-1}{}_{wwt}]$	O
$Cwater_{\text{process water}}$	concentration of substance in surface water after emission of process water via STP	$[kg_c.m^{-3}]$	O
$Cwater_{\text{run-off}}$	concentration of substance in surface water due to run-off	$[kg_c.m^{-3}]$	O
$Cwater_{\text{total}}$	concentration of substance in surface water	$[kg_c.m^{-3}]$	O

Table III-61 Default settings for storage site at automated spraying facility.

Parameter	**Symbol**	**Unit**	**Value**
Duration of storage of treated wood prior to shipment	Tstorage	[d]	3
Volume of wood treated per day			
small company	$V_{\text{wood-treated}}$	$[m^3.d^{-1}]$	52,5
large company			525
Storage density of treated wood on storage area	$D_{\text{wood-stacked}}$	$[m^3.m^{-2}]$	2
Depth of soil	DEPTHsoil	[m]	0.5
Wet soil bulk density	RHO_{soil}	$[kg_{wwt}.m^3]$	1700
Average daily flux of the active ingredient during storage period	$FLUX_{\text{storage}}$	$[kg_c.m^{-2}.d^{-1}]$	-
Effective surface area of treated wood exposed to rain per unit of storage area	$AREA_{\text{wood-exposed}}$	$[m^2.m^{-2}]$	11
Fraction of rain water running of storage area	F_{runoff}	[-]	0.5
Duration of the initial assessment period	$Temission_{\text{ini}}$	[d]	30
Duration of the chronic assessment period	$Temisision_{\text{chron}}$	[d]	>30
Volume flow rate of creek	$FLOW_{\text{creek}}$	$[m^3.d^{-1}]$	25 920

III.3.6.6.2 Scenario for wood preservation through dipping and immersion processes

Parameters/variables and default values for dipping and immersion processes at saw mills, the joinery industry and carpentry shops.

solid application rate: $$Q_{a.i.} = Qform \cdot F_{a.i.} \tag{98}$$

fluid application rate: $$Q_{a.i.} = Vform \cdot RHOform.F_{a.i.} \tag{99}$$

$$Elocal_{3,air} = Q_{a.i.} \cdot VOLUME_{wood-treated} \cdot F_{3,air} \tag{100}$$

$$Elocal_{3,water} = Q_{a.i.} \cdot VOLUME_{wood-treated} \cdot F_{3,water} \tag{101}$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	Temission$_3$	[d]	50
RIVERFLOW	FLOW$_{surfacewater}$	[m^3.d^{-1}]	25920

Input			
VOLUME$_{wood\text{-}treated}$	volume of wood treated per day	[m^3.d^{-1}]	D
VP	vapour pressure	[Pa]	S
SOL	water solubility	[kg$_c$.m^{-3}]	S
F$_{3,air}$	fraction released to air	[-]	O^c
F$_{3,water}$	fraction released to waste water	[-]	O^c
Qform	solid application rate of applied formulation	[kg.m^{-3}]	S
Vform	fluid application rate of applied formulation	[m^3.m^{-3}]	S
RHOproduct	density of product	[kg.m^{-3}]	S
F$_{a.i.}$	fraction of active ingredient in formulation	[-]	S
Temission$_3$	number of emission days for industrial use (including storage)	[d]	D
Output			
Q$_{a.i.}$	quantity of active ingredient applied per m^3 of wood	[kg.m^{-3}]	S/O
Elocal$_{3,water}$	local emission to waste water	[kg$_c$.d^{-1}]	O
Elocal$_{3,air}$	local emission to air during episode	[kg$_c$.d^{-1}]	O

Table III-62 Default settings for dipping and immersion processes.

Parameter	**Symbol**	**Unit**	**Value**
Volume of wood treated per day	$VOLUME_{wood\text{-}treated}$	$[m^3.d^{-1}]$	100
Quantity of active ingredient applied per unit of wood-volume	Q_{ai}	$[kg.m^{-3}]$	-
Fraction released to waste water *Solubility in water [mg.m^{-3}]*	$F_{3,water}$	[-]	
<0.25			0.0001
0.25 – 1			0.0015
1 – 50			0.003
50-100			0.015
≥ 100			0.03
Fraction released to air *Vapour pressure at 20 °C [Pa]*	$F_{3,air}$	[-]	
<0.005			0.001
0.005 - 0.05			0.01
0.05 - 0.5			0.02
0.5 - 1.25			0.075
1.25 - 2.5			0.15
≥2.5			0.25

Parameters/variables and default values for storage at saw mills and carpentry shops, no storage at joinery industry.

In the EUSES 2.1.1 program the concentration of substance in surface water after emissionof process water via STP and due to run-off are presented separately. The concentration in surface water after emission of process water via an STP is presented in the sheet on locan concentration and depositions.

$$AREA_{storage} = \frac{Tstorage \cdot V_{wood-treated}}{D_{wood-stacked}} \qquad \textbf{(102)}$$

$$Qsoil = AREA_{storage} \cdot DEPTHsoil \cdot RHOsoil \qquad \textbf{(103)}$$

$$Elocal_{storage,soil} = FLUX_{storage} \cdot AREA_{wood-exposed} .AREA_{storage} \cdot (1 - F_{runoff}) \qquad \textbf{(104)}$$

$$Csoil_{ini} = \frac{Elocal_{storage,soil} \cdot Temission_{ini}}{Qsoil} \qquad \textbf{(105)}$$

$$Csoil_{chron} = \frac{Elocal_{storage,soil} \cdot Temission_{chron}}{Qsoil} \qquad \textbf{(106)}$$

$$Elocal_{3,surface\ water} = FLUX_{storage} \cdot AREA_{wood-exposed} . AREA_{storage} \cdot F_{runoff} \qquad \textbf{(107)}$$

$$Cwater_{run-off} = \frac{Elocal_{storage,water}}{FLOW_{surfacewater}} \qquad \textbf{(108)}$$

$$Cwater_{processwater} = \frac{Clocal_{eff} \cdot EFFLUENTlocal_{stp}}{FLOW_{surfacewater}} \qquad \textbf{(109)}$$

$$Cwater_{total} = \frac{Elocal_{storage,water}}{FLOW_{surfacewater}} + \frac{Clocal_{eff} \cdot EFFLUENTlocal_{stp}}{FLOW_{surfacewater}} \qquad \textbf{(110)}$$

Input			
Tstorage	duration of storage of treated wood prior to shipment	[d]	D
$V_{wood\text{-}treated}$	volume of wood treated per day	[$m^3.d^{-1}$]	D
$D_{wood\text{-}stacked}$	storage density of treated wood stacked on storage area	[$m^3.m^{-2}$]	D
DEPTHsoil	depth of soil	[m]	D
RHOsoil	wet soil bulk density	[$kg_{wwt}.m^{-3}$]	O^c
$FLUX_{storage}$	average daily flux of the active ingredient during the storage period	[$kg_c.m^{-2}.d^{-1}$]	S
$AREA_{wood\text{-}exposed}$	effective surface area of treated wood exposed to rain per unit of storage area	[$m^2.m^{-2}$]	D
F_{runoff}	fraction of rainwater running off the storage site	[-]	D
$Temission_{ini}$	duration of the initial assessment period	[d]	D
$Temission_{chron}$	duration of the chronic assesssment period	[d]	S
$FLOW_{surfacewater}$	volume flow rate of creek/river	[$m^3.d^{-1}$]	D
$Clocal_{eff}$	concentration in effluent of the local sewage treatment plant	[$kg_c.d^{-1}$]	O^c
$EFFLUENTlocal_{stp}$	effluent flow of the local sewage treatment plant	[$m^3.d^{-1}$]	O^c
Output			
$AREA_{storage}$	surface area of the storage place	[m^2]	D/O
Qsoil	wet soil mass	[kg_{wwt}]	O
$Elocal_{storage,soil}$	local emission to soil from storage	[$kg_c.d^{-1}$]	O
$Elocal_{storage,surface\ water}$	local emission to surface water from storage	[$kg_c.d^{-1}$]	O
$Csoil_{ini}$	concentration of substance in soil for initial assessment period	[$kg_c.kg^{-1}{}_{wwt}$]	O
$Csoil_{chron}$	concentration of substance in soil for longer assessment period	[$kg_c.kg^{-1}{}_{wwt}$]	O
$Cwater_{process\ water}$	concentration of substance in surface water after emission of process water via STP	[$kg_c.m^{-3}$]	O
$Cwater_{run\text{-}off}$	concentration of substance in surface water due to run-off	[$kg_c.m^{-3}$]	O
$Cwater_{total}$	concentration of substance in surface water	[$kg_c.m^{-3}$]	O

Table III-63 Default settings for storage site at saw mills and carpentry shops.

Parameter	**Symbol**	**Unit**	**Value**
Duration of storage of treated wood prior to shipment	Tstorage	[d]	14
Volume of wood treated per day	$V_{wood\text{-}treated}$	$[m^3.d^{-1}]$	100
Storage density of treated wood on storage area	$D_{wood\text{-}stacked}$	$[m^3.m^{-2}]$	2
Surface area of the storage place	$AREA_{storage}$	$[m^{-2}]$	700
Depth of soil	DEPTHsoil	[m]	0.5
Wet soil bulk density	RHO_{soil}	$[kg_{wwt}.m^3]$	1700
Average daily flux of the active ingredient during storage period	$FLUX_{storage}$	$[kg_c.m^{-2}.d^{-1}]$	-
Effective surface area of treated wood exposed to rain per unit of storage area	$AREA_{wood\text{-}leach}$	$[m^2.m^{-2}]$	11
Fraction of rain water running of storage area	F_{runoff}	[-]	0.5
Duration of the initial assessment period	$Temission_{ini}$	[d]	30
Duration of the chronic assessment period	$Temisision_{chron}$	[d]	>30
Volume flow rate of creek	$FLOW_{surfacewater}$	$[m^3.d^{-1}]$	25920

.3.5.1. *Scenario for wood preservation through Vacuum-Pressure and Double- Vacuum/Low Pressure processes*

Parameters/variables and default values for V-P and D-V/LP processes.

solid application rate: $$Q_{a.i.} = Qform \cdot F_{a.i.} \quad \textbf{(111)}$$

fluid application rate: $$Q_{a.i.} = Vform \cdot RHOform.F_{a.i.} \quad \textbf{(112)}$$

$$Elocal_{3,water} = Q_{a.i.} \cdot AREA_{wood-treated} \cdot F_{3,air} \quad \textbf{(113)}$$

$$Elocal_{3,air} = Q_{a.i.} \cdot AREA_{wood-treated} \cdot F_{3,water} \quad \textbf{(114)}$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_3$	[d]	250
RIVERFLOW	$FLOW_{surfacewater}$	$[m^3.d^{-1}]$	25920

Input			
$VOLUME_{wood\text{-}treated}$	volume of wood treated per day	$[m^3.d^{-1}]$	D
VP	vapour pressure	[Pa]	S
SOL	water solubility	$[kg_c.m^{-3}]$	S
$F_{3,air}$	fraction released to air	[-]	O^c
$F_{3,water}$	fraction released to waste water	[-]	O^c
Qform	solid application rate of applied formulation	$[kg.m^{-3}]$	S
Vform	fluid application rate of applied formulation	$[m^3.m^{-3}]$	S
RHOproduct	density of product	$[kg.m^{-3}]$	S
$F_{a.i.}$	fraction of active ingredient in formulation	[-]	S
$Temission_3$	number of emission days for industrial use (including storage)	[d]	D
Output			
$Q_{a.i.}$	quantity of active ingredient applied per m^3 of wood	$[kg.m^{-3}]$	S/O
$Elocal_{3,water}$	local emission to waste water	$[kg_c.d^{-1}]$	O
$Elocal_{3,air}$	local emission to air during episode	$[kg_c.d^{-1}]$	O

Table III-64 Default settings for dipping and immersion processes.

Parameter	**Symbol**	**Unit**	**Value**
Volume of wood treated per day	$VOLUME_{treated\text{-}wood}$	$[m^3.d^{-1}]$	
- vacuum pressure			30
- double vacuum			15
Quantity of active ingredient applied per unit of wood-volume	Q_{ai}	$[kg.m^{-3}]$	-
Fraction released to waste water *Solubility in water [mg.m^{-3}]*	$F_{3,water}$	[-]	
<0.25			0.0001
0.25 – 1			0.0015
1 – 50			0.003
50-100			0.015
≥ 100			0.03
Fraction released to air *Vapour pressure at 20 °C [Pa]*	$F_{3,air}$	[-]	
<0.005			0.001
0.005 - 0.05			0.01
0.05 - 0.5			0.02
0.5 - 1.25			0.075
1.25 - 2.5			0.15
≥2.5			0.25

Parameters/variables and default values for storage at vacuum-pressure treatment.
In the EUSES 2.1.1 program the concentration of substance in surface water after emissionof process water via STP and due to run-off are presented separately. The concentration in surface water after emission of process water via an STP is presented in the sheet on locan concentration and depositions.

$$AREA_{storage} = \frac{Tstorage \cdot V_{wood-treated}}{D_{wood-stacked}} \tag{115}$$

$$Qsoil = AREA_{storage} \cdot DEPTHsoil \cdot RHOsoil \tag{116}$$

$$Elocal_{storage,soil} = FLUX_{storage} \cdot AREA_{wood-exposed} .AREA_{storage} \cdot (1 - F_{runoff}) \tag{117}$$

$$Csoil_{ini} = \frac{Elocal_{storage,soil} \cdot Temission_{ini}}{Qsoil} \tag{118}$$

$$Csoil_{chron} = \frac{Elocal_{storage,soil} \cdot Temission_{chron}}{Qsoil} \tag{119}$$

$$Elocal_{3,surface\ water} = FLUX_{storage} \cdot AREA_{wood-exposed} .AREA_{storage} \cdot F_{runoff} \tag{120}$$

$$Cwater_{run-off} = \frac{Elocal_{storage,water}}{FLOW_{surfacewater}} \tag{121}$$

$$Cwater_{processwater} = \frac{Clocal_{eff} \cdot EFFLUENTlocal_{stp}}{FLOW_{surfacewater}} \tag{122}$$

$$Cwater_{total} = \frac{Elocal_{storage,water}}{FLOW_{surfacewater}} + \frac{Clocal_{eff} \cdot EFFLUENTlocal_{stp}}{FLOW_{surfacewater}} \tag{123}$$

Input			
Tstorage	duration of storage of treated wood prior to shipment	[d]	D
$V_{wood-treated}$	volume of wood treated per day	[$m^3.d^{-1}$]	D
$D_{wood-stacked}$	storage density of treated wood stacked on storage area	[$m^3.m^{-2}$]	D
DEPTHsoil	depth of soil	[m]	D
RHOsoil	wet soil bulk density	[$kg_{wwt}.m^{-3}$]	O^c
$FLUX_{storage}$	average daily flux of the active ingredient during the storage period	[$kg_c.m^{-2}.d^{-1}$]	S
$AREA_{wood-exposed}$	effective surface area of treated wood exposed to rain per unit of storage area	[$m^2.m^{-2}$]	D
F_{runoff}	fraction of rainwater running off the storage site	[-]	D
$Temission_{ini}$	duration of the initial assessment period	[d]	D
$Temission_{chron}$	duration of the chronic assesssment period	[d]	S
$Clcoal_{eff}$	local treatment plant effluent concentration	[$kg_c.m^{-3}$]	O^c
$EFFLUENTlocal_{stp}$	effluent flow of the local sewage treatment plant	[$m^3.d^{-1}$]	O^c
$FLOW_{surfacewater}$	volume flow rate of creek	[$m^3.d^{-1}$]	D
Output			
$AREA_{storage}$	surface area of the storage place	[m^2]	D/O
Qsoil	wet soil mass	[kg_{wwt}]	O
$Elocal_{3,soil}$	local emission to soil from storage	[$kg_c.d^{-1}$]	O
$Elocal_{3,surface\ water}$	local emission to surface water from storage	[$kg_c.d^{-1}$]	O
$Csoil_{ini}$	concentration of substance in soil for initial assessment period	[$kg_c.kg^{-1}{}_{wwt}$]	O
$Csoil_{chron}$	concentration of substance in soil for longer assessment period	[$kg_c.kg^{-1}{}_{wwt}$]	O
$Cwater_{process\ water}$	concentration of substance in surface water after emission of process water via STP	[$kg_c.m^{-3}$]	O
$Cwater_{run-off}$	concentration of substance in surface water due to run-off	[$kg_c.m^{-3}$]	O
$Cwater_{total}$	concentration of substance in surface water	[$kg_c.m^{-3}$]	O

Table III-65 Default settings for storage site at vacuum-pressure treatment.

Parameter	**Symbol**	**Unit**	**Value**
Duration of storage of treated wood prior to shipment	Tstorage	[d]	35
Volume of wood treated per day	$V_{wood\text{-}treated}$	$[m^3.d^{-1}]$	
- vacuum pressure			30
- double vacuum			15
Storage density of treated wood on storage area	$D_{wood\text{-}stacked}$	$[m^3.m^{-2}]$	2
Surface area of the storage place	$AREA_{sttorage}$	$[m^{-2}]$	
- vacuum pressure			525
- double vacuum			263
Depth of soil	DEPTHsoil	[m]	0.5
Wet soil bulk density	RHO_{soil}	$[kg_{wwt}.m^3]$	1700
Average daily flux of the active ingredient during storage period	$FLUX_{storage}$	$[kg_c.m^{-2}.d^{-1}]$	-
Effective surface area of treated wood exposed to rain per unit of storage area	$AREA_{wood\text{-}leach}$	$[m^2.m^{-2}]$	11
Fraction of rain water running of storage area	F_{runoff}	[-]	0.5
Duration of the initial assessment period	$Temission_{ini}$	[d]	30
Duration of the chronic assessment period	$Temisision_{chron}$	[d]	>30
Volume flow rate of creek	$FLOW_{surfacewater}$	$[m^3.s^{-1}]$	25920

.3.5.2. *Calculation of soil concentrations taking degradation into account*

Parameters/variables and default values for <u>storage</u>, taking degradation into account.

Removal from soil:

$$Csoil_{ss} = \frac{Elocal_{3,soil}}{Qsoil} \cdot \frac{1}{k_{soil}} \qquad \textbf{(124)}$$

$$Csoil_{pore} = \frac{Csoil_{ss} \cdot RHOsoil}{K_{soil-water}} \qquad \textbf{(125)}$$

Input			
RHOsoil	wet soil bulk density	$[kg_{wwt}.m^{-3}]$	O^c
Qsoil	wet soil mass	$[kg_{wwt}]$	O
$Elocal_{3,soil}$	local emission to soil from storage	$[kg_c.d^{-1}]$	O
Ksoil-water	soil-water equilibrium distribution coefficient	$[m^3_{water}.m^{-3}_{soil}]$	O
k_{soil}	first-order rate constant for removal from soil	$[d^{-1}]$	S
Output			
$Csoil_{ss}$	steady-state concentration in soil	$[kg_c.kg^{-1}_{wwt}]$	O
$Csoil_{pore}$	steady state concentration in soil pore water	$[kg_c.m^{-3}]$	O

Service Life

III.3.6.6.3 Emissions from treated wood, scenario for a fence

Parameters/variables and default values for a fence.

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_{ini}$	[d]	30
Temission	$Temission_{chron}$	[d]	>30

$$Vsoil = 1 \cdot WIDTHsoil \cdot DEPTHsoil \tag{126}$$

$$Qsoil = Vsoil \cdot RHOsoil \tag{127}$$

$$Qleach_{ini} = FLUX_{wood,ini} \cdot AREA_{fence} \tag{128}$$

$$Qleach_{chron} = FLUX_{wood,chron} \cdot AREA_{fence} \tag{129}$$

$$Csoil_{ini} = \frac{Qleach_{ini} \cdot Temission_{ini}}{Qsoil} \tag{130}$$

$$Csoil_{chron} = \frac{Qleach_{chron} \cdot Temission_{chron}}{Qsoil} \tag{131}$$

Input

WIDTHsoil	width of receiving soil	[m]	D
DEPTHsoil	depth of receiving soil	[m]	D
Vsoil	volume of soil	[m^3]	O
RHOsoil	wet soil bulk density	[$kg_{wwt}.m^{-3}$]	D
$FLUX_{wood,ini}$	average daily flux of the active ingredient over the initial assessment period	[$kg_c.m^{-2}.d^{-1}$]	S
$FLUX_{wood,chron}$	average daily flux of the active ingredient over the chronic assessment period	[$kg_c.m^{-2}.d^{-1}$]	S
$AREA_{fence}$	leachable wood area per unit of length of fence	[m^2]	D

Output

Qsoil	wet soil mass	[kg_{wwt}]	O/S
$Qleach_{ini}$	average rate of active ingredient leached out of treated wood during the initial assessment period	[$kg_c.d^{-1}$]	O/S
$Qleach_{chron}$	average rate of active ingredient leached out of treated wood during the chronic assessment period	[$kg_c.d^{-1}$]	O
$Csoil_{ini}$	concentration of substance in soil for initial assessment period	[$kg_c.kg^{-1}{}_{wwt}$]	O
$Csoil_{chron}$	concentration of substance in soil for longer assessment period	[$kg_c.kg^{-1}{}_{wwt}$]	O

Table III-66 Default settings for the fence scenario.

Parameter	**Symbol**	**Unit**	**Value**
Leachable surface area of the fence per unit of length	$AREA_{fence}$	[m^2]	2
Width of receiving soil compartment	WIDTHsoil	[m]	0.5
Depth of receiving soil compartment	DEPTHsoil	[m]	0.5
Wet soil bulk density	RHO_{soil}	[$kg_{wwt}.m^3$]	1700

III.3.6.6.4 Emissions from treated wood, scenario for a noise barrier

Parameters/variables and default values for a noise barrier.

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_{ini}$	[d]	30
Temission	$Temission_{chron}$	[d]	>30

$$Vsoil = 1000 \cdot WIDTHsoil \cdot DEPTHsoil \quad \textbf{(132)}$$

$$Qsoil = Vsoil \cdot RHOsoil \quad \textbf{(133)}$$

$$Qleach_{ini} = FLUX_{wood,ini} \cdot AREA_{noise\ barrier} \quad \textbf{(134)}$$

$$Qleach_{chron} = FLUX_{wood,chron} \cdot AREA_{noise\ barrier} \quad \textbf{(135)}$$

$$Csoil_{ini} = \frac{Qleach_{ini} \cdot Temission_{ini} \cdot F_{soil}}{Qsoil} \quad \textbf{(136)}$$

$$Csoil_{chron} = \frac{Qleach_{chron} \cdot Temission_{chron} \cdot F_{soil}}{Qsoil} \quad \textbf{(137)}$$

$$Elocal\_ini_{4,water} = FLUX_{wood,ini} \cdot AREA_{noise\ barrier} . \cdot F_{4,water} \quad \textbf{(138)}$$

$$Elocal\_chron_{4,water} = FLUX_{wood,chron} \cdot AREA_{noise\ barrier} . \cdot F_{4,water} \quad \textbf{(139)}$$

Input

WIDTHsoil	width of receiving soil	[m]	D
DEPTHsoil	depth of receiving soil	[m]	D
Vsoil	volume of soil	[m^3]	O
RHOsoil	wet soil bulk density	[$kg_{wwt}.m^{-3}$]	D
$FLUX_{wood,ini}$	average daily flux of the active ingredient over the initial assessment period	[$kg_c.m^{-2}.d^{-1}$]	S
$FLUX_{wood,chron}$	average daily flux of the active ingredient over the chronic assessment period	[$kg_c.m^{-2}.d^{-1}$]	S
$AREA_{noise\ barrier}$	leachable wood area for noise barrier	[m^2]	D
F_{soil}	fraction of substance leached to soil	[-]	D
$F_{4,water}$	fraction of substance leached to waste water	[-]	D

Output

Qsoil	wet soil mass	[kg_{wwt}]	O
$Qleach_{ini}$	average rate of active ingredient leached out of treated wood for the initial assessment period	[$kg_c.d^{-1}$]	O/S
$Qleach_{chron}$	average rate of active ingredient leached from treated wood for the chronic assessment period	[$kg_c.d^{-1}$]	O/S
$Csoil_{ini}$	concentration of substance in soil for initial assessment period	[$kg_c.kg^{-1}{}_{wwt}$]	O
$Csoil_{chron}$	concentration of substance in soil for longer assessment period	[$kg_c.kg^{-1}{}_{wwt}$]	O
$Elocal\_ini_{4,water}$	local emission to waste water for the initial assessment period	[$kg_c.kg^{-1}{}_{wwt}$]	O
$Elocal\_chron_{4,water}$	local emission to waste water for the chronic assessment period	[$kg_c.kg^{-1}{}_{wwt}$]	O

Table III-67 Default settings for the noise barrier scenario.

Parameter	**Symbol**	**Unit**	**Value**
Leachable surface area of the noise barrier	$AREA_{noise\ barrier}$	[m^2]	3000
Distance from fence, witdth receiving soil	WIDTH	[m]	0.5
Depth of receiving soil	DEPTHsoil	[m]	0.5
Wet soil bulk density	RHO_{soil}	[$kg_{wwt}.m^3$]	1700
Fraction of substance leached to soil	F_{soil}	[-]	0.3
Fraction of substance leached to water	$F_{4,water}$	[-]	0.7

III.3.6.6.5 Emissions from treated wood, scenario for a wooden house

Parameters/variables and default values for a fence.

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_{ini}$	[d]	30
Temission	$Temission_{chron}$	[d]	>30

$$Vsoil = [(7.5 + 2 \cdot WIDTHsoil) \cdot (17.5 + 2 \cdot WIDTHsoil) - (7.5 \cdot 17.5)] \cdot DEPTHsoil \quad \textbf{(140)}$$

$$Qsoil = Vsoil \cdot RHOsoil \quad \textbf{(141)}$$

$$Qleach_{ini} = FLUX_{wood,ini} \cdot AREA_{house} \quad \textbf{(142)}$$

$$Qleach_{chron} = FLUX_{wood,chron} \cdot AREA_{house} \quad \textbf{(143)}$$

$$Csoil_{ini} = \frac{Qleach_{ini} \cdot Temission_{ini}}{Qsoil} \quad \textbf{(144)}$$

$$Csoil_{chron} = \frac{Qleach_{chron} \cdot Temission_{chron}}{Qsoil} \quad \textbf{(145)}$$

Input			
WIDTHsoil	width of receiving soil	[m]	D
DEPTHsoil	depth of receiving soil	[m]	D
Vsoil	volume of soil	[m^3]	O
RHOsoil	wet soil bulk density	[$kg_{wwt}.m^{-3}$]	D
$FLUX_{wood,ini}$	average daily flux of the active ingredient over the initial assessment period	[$kg_c.m^{-2}.d^{-1}$]	S
$FLUX_{wood,chron}$	average daily flux of the active ingredient over the chronic assessment period	[$kg_c.m^{-2}.d^{-1}$]	S
$AREA_{house}$	leachable area of the wooden house	[m^2]	D
Output			
Qsoil	wet soil mass	[kg_{wwt}]	O/S
$Qleach_{ini}$	average rate of active ingredient leached out of treated wood during the initial assessment period	[$kg_c.d^{-1}$]	O/S
$Qleach_{chron}$	average rate of active ingredient leached out of treated wood during the chronic assessment period	[$kg_c.d^{-1}$]	O
$Csoil_{ini}$	concentration of substance in soil for initial assessment period	[$kg_c.kg^{-1}_{wwt}$]	O
$Csoil_{chron}$	concentration of substance in soil for longer assessment period	[$kg_c.kg^{-1}_{wwt}$]	O

Table III-68 Default settings for the wooden house scenario.

Parameter	**Symbol**	**Unit**	**Value**
Leachable surface area of the wooden house	$AREA_{fence}$	[m^2]	125
Width soil, distance from the house	WIDTH	[m]	0.5
Depth of soil	DEPTHsoil	[m]	0.5
Wet soil bulk density	RHO_{soil}	[$kg_{wwt}.m^3$]	1700

III.3.6.6.6 Emissions from treated wood, scenario for a transmission pole

Parameters/variables and default values for a transmission pole.

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_{ini}$	[d]	30
Temission	$Temission_{chron}$	[d]	>30

$$Vsoil = (2 + DEPTHsoil) \cdot \pi \cdot (0.125 + WIDTHsoil)^2 - 2 \cdot \pi \cdot 0.125^2 \tag{146}$$

$$Qsoil = Vsoil \cdot RHOsoil \tag{147}$$

$$Qleach_{ini} = FLUX_{wood,ini} \cdot (AREA_{pole,above} + AREA_{pole,below}) \tag{148}$$

$$Qleach_{chron} = FLUX_{wood,chron} \cdot (AREA_{pole,above} + AREA_{pole,below}) \tag{149}$$

$$Csoil_{ini} = \frac{Qleach_{ini} \cdot Temission_{ini}}{Qsoil} \tag{150}$$

$$Csoil_{chron} = \frac{Qleach_{chron} \cdot Temission_{chron}}{Qsoil} \tag{151}$$

Input			
WIDTHsoil	width of receiving soil	[m]	D
DEPTHsoil	depth of receiving soil	[m]	D
Vsoil	volume of soil	[m^3]	O
RHOsoil	wet soil bulk density	[$kg_{wwt}.m^{-3}$]	D
$FLUX_{wood,ini}$	average daily flux of the active ingredient over the initial assessment period	[$kg_c.m^{-2}.d^{-1}$]	S
$FLUX_{wood,chron}$	average daily flux of the active ingredient over the chronic assessment period	[$kg_c.m^{-2}.d^{-1}$]	S
$AREA_{pole,above}$	leachable area of the wooden pole above ground	[m^2]	D
$AREA_{pole,below}$	leachable area of the wooden pole below ground	[m^2]	D
Output			
Qsoil	wet soil mass	[kg_{wwt}]	O/S
$Qleach_{ini}$	average rate of active ingredient leached out of treated wood during the initial assessment period	[$kg_c.d^{-1}$]	O/S
$Qleach_{chron}$	average rate of active ingredient leached out of treated wood during the chronic assessment period	[$kg_c.d^{-1}$]	O
$Csoil_{ini}$	concentration of substance in soil for initial assessment period	[$kg_c.kg^{-1}_{wwt}$]	O
$Csoil_{chron}$	concentration of substance in soil for longer assessment period	[$kg_c.kg^{-1}_{wwt}$]	O

Table III-69 Default settings for the transmission pole scenario.

Parameter	**Symbol**	**Unit**	**Value**
Leachable surface area of the wooden pole above ground	$AREA_{pole,above}$	[m^2]	5.5
Leachable surface area of the wooden pole below ground	$AREA_{pole,below}$	[m^2]	1.6
Width of soil, distance from pole	WITDHsoil	[m]	0.5
Depth of soil under pole	DEPTHsoil	[m]	0.5
Wet soil bulk density	RHO_{soil}	[kg_{wwt}.m^3]	1700

III.3.6.6.7 Emissions from treated wood, scenario for a fence post

Parameters/variables and default values for a fence post.

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_{ini}$	[d]	30
Temission	$Temission_{chron}$	[d]	>30

$$Vsoil = (0.5 + DEPTHsoil) \cdot (0.1 + 2 \cdot WIDTHsoil)^2 - 0.5 \cdot 0.1^2 \qquad \textbf{(152)}$$

$$Qsoil = Vsoil \cdot RHOsoil \qquad \textbf{(153)}$$

$$Qleach_{ini} = FLUX_{wood,ini} \cdot (AREA_{post,above} + AREA_{post,below}) \qquad \textbf{(154)}$$

$$Qleach_{chron} = FLUX_{wood,chron} \cdot (AREA_{post,above} + AREA_{post,below}) \qquad \textbf{(155)}$$

$$Csoil_{ini} = \frac{Qleach_{ini} \cdot Temission_{ini}}{Qsoil} \qquad \textbf{(156)}$$

$$Csoil_{chron} = \frac{Qleach_{chron} \cdot Temission_{chron}}{Qsoil} \qquad \textbf{(157)}$$

Input

WIDTHsoil	width of receiving soil	[m]	D
DEPTHsoil	depth of receiving soil	[m]	D
Vsoil	volume of soil	[m^3]	O
RHOsoil	wet soil bulk density	[$kg_{wwt}.m^{-3}$]	D
$FLUX_{wood,ini}$	average daily flux of the active ingredient over the initial assessment period	[$kg_c.m^{-2}.d^{-1}$]	S
$FLUX_{wood,chron}$	average daily flux of the active ingredient over the chronic assessment period	[$kg_c.m^{-2}.d^{-1}$]	S
$AREA_{post,above}$	leachable area of the fence post above ground	[m^2]	D
$AREA_{post,below}$	leachable area of the fence post below ground	[m^2]	D

Output

Qsoil	wet soil mass	[kg_{wwt}]	O/S
$Qleach_{ini}$	average rate of active ingredient leached out of treated wood during the initial assessment period	[$kg_c.d^{-1}$]	O/S
$Qleach_{chron}$	average rate of active ingredient leached out of treated wood during the chronic assessment period	[$kg_c.d^{-1}$]	O
$Csoil_{ini}$	concentration of substance in soil for initial assessment period	[$kg_c.kg^{-1}{}_{wwt}$]	O
$Csoil_{chron}$	concentration of substance in soil for longer assessment period	[$kg_c.kg^{-1}{}_{wwt}$]	O

Table III-70 Default settings for the fence post scenario.

Parameter	Symbol	Unit	Value
Leachable surface area of the fence post above ground	$AREA_{post,above}$	[m^2]	0.8
Leachable surface area of the fence post below ground	$AREA_{post,below}$	[m^2]	0.2
Width of soil compartment, distance from post	WITDHsoil	[m]	0.5
Depth of soil under post	DEPTHsoil	[m]	0.5
Wet soil bulk density	RHO_{soil}	[$kg_{wwt}.m^3$]	1700

III.3.6.6.8 Emissions from treated wood, scenario for a jetty in a lake

Parameters/variables and default values for a jetty.

Parameters required for distribution modules	Defaults for this scenario	Unit	Value
Temission	$Temission_{ini}$	[d]	30
Temission	$Temission_{chron}$	[d]	>30

$$Qleach_{ini} = FLUX_{wood,ini} \cdot (AREA_{planks} + AREA_{poles}) \tag{158}$$

$$Qleach_{chron} = FLUX_{wood,chron} \cdot (AREA_{planks} + AREA_{poles}) \tag{159}$$

$$Cwater_{ini} = \frac{Qleach_{ini} \cdot Temission_{ini}}{Vwater} \tag{160}$$

$$Cwater_{chron} = \frac{Qleach_{chron} \cdot Temission_{chron}}{Vwater} \tag{161}$$

Input			
Vwater	volume of water	[m^3]	D
$FLUX_{wood,ini}$	average daily flux of the active ingredient over the initial assessment period	[$kg_c.m^{-2}.d^{-1}$]	S
$FLUX_{wood,chron}$	average daily flux of the active ingredient over the chronic assessment period	[$kg_c.m^{-2}.d^{-1}$]	S
$AREA_{planks}$	leachable area of the jetty planks	[m^2]	D
$AREA_{poles}$	leachable area of the jetty poles	[m^2]	D
Output			
$Qleach_{ini}$	average rate of active ingredient leached out of treated wood during the initial assessment period	[$kg_c.d^{-1}$]	O/S
$Qleach_{chron}$	average rate of active ingredient leached out of treated wood during the chronic assessment period	[$kg_c.d^{-1}$]	O
$Cwater_{ini}$	local concentration in water at the end of the initial assessment period	[$kg_c.m^{-3}$]	O
$Cwater_{chron}$	local concentration in water at the end of the longer assessment period	[$kg_c.m^{-3}$]	O

Table III-71 Default settings for the jetty in lake scenario.

Parameter	**Symbol**	**Unit**	**Value**
Leachable surface area of the jetty planks	$AREA_{planks}$	[m^2]	16.2
Leachable surface area of the jetty poles	$AREA_{poles}$	[m^2]	10.0
Volume of water	Vwater	[m^3]	16,000

III.3.6.6.9 Emissions from treated wood, scenario for a sheet piling in a waterway

Parameters/variables and default values for a sheet piling.

$$Qleach_{ini} = FLUX_{wood,ini} \cdot AREA_{piling} \quad \textbf{(162)}$$

$$Qleach_{chron} = FLUX_{wood,chron} \cdot AREA_{piling} \quad \textbf{(163)}$$

$$Cwater_{ini} = \frac{Qleach_{ini} \cdot TAU_{wway}}{Vwater} \quad \textbf{(164)}$$

$$Cwater_{chron} = \frac{Qleach_{chron} \cdot TAU_{wway}}{Vwater} \quad \textbf{(165)}$$

Input			
Vwater	volume of water	[m^3]	D
$FLUX_{wood,ini}$	average daily flux of the active ingredient over the initial assessment period	[$kg_c.m^{-2}.d^{-1}$]	S
$FLUX_{wood,chron}$	average daily flux of the active ingredient over the chronic assessment period	[$kg_c.m^{-2}.d^{-1}$]	S
TAU_{wway}	residence time of water in the waterway	[d]	D
$AREA_{piling}$	leachable area of the sheet piling per unit of lenght of waterway	[m^2]	D
Output			
$Qleach_{ini}$	average rate of active ingredient leached out of treated wood during the initial assessment period	[$kg_c.d^{-1}$]	O/S
$Qleach_{chron}$	average rate of active ingredient leached out of treated wood during the chronic assessment period	[$kg_c.d^{-1}$]	O
$Cwater_{ini}$	local concentration in water at the end of the initial assessment period	[$kg_c.m^{-3}$]	O
$Cwater_{chron}$	local concentration in water at the end of the longer assessment period	[$kg_c.m^{-3}$]	O

Table III-72 Default settings for sheet piling scenario.

Parameter	**Symbol**	**Unit**	**Value**
Leachable surface area of the sheet piling per unit of length of waterway	$AREA_{piling}$	[m^2]	4.7
Residence time of water in the waterway	TAU_{wway}	[d]	20
Volume of water	Vwater	[m^3]	7.5

III.3.6.6.10 Emissions from treated wood, scenario for a wharf in salt water

Parameters/variables and default values for a wharf.

A) poles and planks are considered separately

$$Qleach_{ini} = FLUX_{water,ini} \cdot AREA_{planks} + FLUX_{salt\ water,ini} \cdot AREA_{poles} \tag{166}$$

$$Qleach_{chron} = FLUX_{water,chron} \cdot AREA_{planks} + FLUX_{salt\ water,chron} \cdot AREA_{poles} \tag{167}$$

B) poles and planks are considered together, leaching based on test with de-ionised water

$$Qleach_{ini} = FLUX_{water,ini} \cdot (AREA_{planks} + AREA_{poles}) \tag{168}$$

$$Qleach_{chron} = FLUX_{water,chron} \cdot (AREA_{planks} + \cdot AREA_{poles}) \tag{169}$$

A+B)

$$Cwater_{ini} = \frac{Qleach_{ini} \cdot TAU_{wway}}{Vwater} \tag{170}$$

$$Cwater_{chron} = \frac{Qleach_{chron} \cdot TAU_{wway}}{Vwater} \tag{171}$$

Input			
Vwater	volume of water	$[m^3]$	D
$FLUX_{water,ini}$	average daily flux of the active ingredient over the initial assessment period, based on test with de-ionised water	$[kg_c.m^{-2}.d^{-1}]$	S
$FLUX_{water,chron}$	average daily flux of the active ingredient over the chronic assessment period, based on test with de-ionised water	$[kg_c.m^{-2}.d^{-1}]$	S
$FLUX_{salt\ water,ini}$	average daily flux of the active ingredient over the initial assessment period, based on test with simulated sea water	$[kg_c.m^{-2}.d^{-1}]$	S
$FLUX_{salt\ water,chron}$	average daily flux of the active ingredient over the chronic assessment period, based on test with simulated sea water	$[kg_c.m^{-2}.d^{-1}]$	S
$TAU_{seawater}$	residence time of water in the waterway	[d]	D
$AREA_{poles}$	leachable area of the wharf poles	$[m^2]$	D
$AREA_{planks}$	leachable area of the wharf planks	$[m^2]$	D
Output			
$Qleach_{ini}$	average rate of active ingredient leached out of treated wood during the initial assessment period	$[kg_c.d^{-1}]$	O
$Qleach_{chron}$	average rate of active ingredient leached out of treated wood during the chronic assessment period	$[kg_c.d^{-1}]$	O
$Csea\ water_{ini}$	local concentration in sea water at the end of the initial assessment period	$[kg_c.m^{-3}]$	O
$Csea\ water_{chron}$	local concentration in sea water at the end of the longer assessment period	$[kg_c.m^{-3}]$	O

Table III-73 Default settings for the wharf scenario.

Parameter	**Symbol**	**Unit**	**Value**
Leachable surface area of the wharf poles	$AREA_{poles}$	$[m^2]$	296
Leachable surface area of the wharf planks	$AREA_{planks}$	$[m^2]$	911
Residence time of water in the waterway	TAU_{wway}	[d]	0.5
Volume of water	Vwater	$[m^3]$	1000

Professional and private use, non industrial

III.3.6.6.11 Wood preservatives used in indoors curative and preventive treatments, fumigation (professional use only)

The model for curative and preventive wood treatment through indoor fumigation, the input for the biocide has to be specified as the amount for a single application.

$$Elocal_{air} = \frac{Vtreat \cdot Q_{subst} \cdot (1 - F_{ret}) \cdot (1 - F_{disin})}{1} \qquad \textbf{(172)}$$

(the 1 in the formula is one day of the emission episode)

Input

Q_{subst}	amount of active ingredient used	[kg.m^{-3}]	S
V_{treat}	treated volume	[m^3]	S
F_{ret}	fraction of retention in goods	[-]	D
F_{disin}	fraction of disintegration	[-]	D
$Temission_{fogging}$	number of emission days for fogging	[d]	S
Output			
$Elocal_{air}$	local emission to air during episode	[kg.d^{-1}]	O
Temission	number of emission days		

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_{fogging}$	[d]	1

Table III-74 Default settings for calculating releases from indoors applications, fumigation

Parameter	**Symbol**	**Unit**	**Value**
Treated volume	Vtreat	[m^3]	
chamber/container			100
small room (e.g. museum)			300
big volume (e.g. church)			10,000
Fraction of retention in goods	F_{ret}	[-]	0.02
Fraction of disintegration	F_{disin}	[-]	0.001

III.3.6.6.12 Wood preservatives used in curative and preventive outdoor treatments, brushing

Emissions from brushing outdoors for fence, house (only soil) and bridge (only water):

$$\mathrm{Elocal}_{soil,item} = \mathrm{AREA}_{item} \cdot Qprod \cdot Cprod \cdot RHOprod \cdot Fsoil_{brush} \tag{173}$$

$$\mathrm{Elocal}_{water,item} = \mathrm{AREA}_{item} \cdot Qprod \cdot Cprod \cdot RHOprod \cdot Fwater_{brush} \tag{174}$$

$$\mathrm{Clocal}_{soil,brush} = \frac{\mathrm{Elocal}_{soil,brush}}{\mathrm{Vsoil}_{item} \cdot \mathrm{RHOsoil}} \tag{175}$$

$$\mathrm{Clocal}_{water,brush} = \frac{\mathrm{Elocal}_{water,brush}}{\mathrm{Vwater}_{item}} \tag{176}$$

Input

$AREA_{item}$	treated wood area per event	[m^2]	D
Q_{prod}	amount of substance used	[$m^3.m^{-2}$]	S
C_{prod}	concentration of ative ingredient in used product	[-]	S
RHOprod	density of applied product	[$kg.m^{-3}$]	S
$Fsoil_{brush}$	fraction of product lost during brushing	[-]	D
$Fwater_{brush}$	fraction of product lost during brushing	[-]	D
$Vsoil_{item}$	volume of contaminated soil	[m^3]	D
$Vwater_{item}$	volume of contaminated water	[m^3]	D
RHOsoil	bulk density of wet soil	[$kg.m^{-3}$]	D

Output

$Elocal_{water,item}$	local emission to water during application	[kg]	O
$Elocal_{soil,item}$	local emission to soil during application	[kg]	O
$Clocal_{water,brush}$	local concentration in water at day one of application	[$kg.m^{-3}$]	O
$Clocal_{soil,bruah}$	local concentration in soil at the end of day one of application	[$kg.kg_{wwt}^{-1}$]	O

Table III-75 Default settings for calculating releases from brushing

Parameter	**Symbol**	**Unit**	**Value**
Treated wood area	AREAitem	[m^2]	
fence			4
house			125
bridge			10
Fraction lost during brushing	$Fsoil_{brush}$	[-]	
professional			0.03
amateur			0.05
Fraction lost during brushing	$Fwater_{brush}$	[-]	
professional			0.03
amateur			0.05
Volume of contimated water	$Vwater_{item}$	[m^3]	
bridge			20
Volume of contaminated soil	$Vsoil_{item}$	[m^3]	
fence			2* equation 129
house			equation 143
Density of soil	RHOsoil	[$kg_{wwt}.m^{-3}$]	1700

Emissions after application, from leaching:

For the fence and house scenarios, the emissions to soil from treated wood can be calculated according to Sections 3.6.17 and 3.6.19 respectively.

Parameters/variables and default values for a bridge.

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_{ini}$	[d]	30
Temission	$Temission_{chron}$	[d]	>30

$$Qleach_{ini} = FLUX_{wood,ini} \cdot AREA_{bridge} \tag{177}$$

$$Qleach_{chron} = FLUX_{wood,chron} \cdot AREA_{bridge} \tag{178}$$

$$Cwater_{ini} = \frac{Qleach_{ini} \cdot Temission_{ini}}{Vwater} \tag{179}$$

$$Cwater_{chron} = \frac{Qleach_{chron} \cdot Temission_{chron}}{Vwater} \tag{180}$$

Input

Vwater	volume of water	$[m^3]$	D
$FLUX_{wood,ini}$	average daily flux of the active ingredient over the initial assessment period	$[kg_c.m^{-2}.d^{-1}]$	S
$FLUX_{wood,chron}$	average daily flux of the active ingredient over the chronic assessment period	$[kg_c.m^{-2}.d^{-1}]$	S
$AREA_{bridge}$	leachable wood area	$[m^2]$	D

Output

$Qleach_{ini}$	average rate of active ingredient leached out of treated wood during the initial assessment period	$[kg_c.d^{-1}]$	O
$Qleach_{chron}$	average rate of active ingredient leached out of treated wood during the chronic assessment period	$[kg_c.d^{-1}]$	O
$Cwater_{leach,ini}$	concentration of substance in water due to leaching, for the initial assessment period	$[kg_c.m^{-3}]$	O
$Cwater_{leach,chron}$	concentration of substance in water due to leaching for the longer assessment period	$[kg_c.m^{-3}]$	O

Table III-76 Default settings for the bridge leaching scenario.

Parameter	**Symbol**	**Unit**	**Value**
Leachable surface area	$AREA_{bridge}$	$[m^2]$	10
Volume of water	Vwater	$[m^3]$	20

Total concentration for each item, fence, house (only soil) and bridge (only water):

$$Clocal_{soil,ini} = Clocal_{soil,brush} + Clocal_{soil,leach,ini} \quad \textbf{(181)}$$

$$Clocal_{water,ini} = Clocal_{water,brush} + Clocal_{water,leach,ini} \quad \textbf{(182)}$$

$$Clocal_{soil,chron} = Clocal_{soil,brush} + Clocal_{soil,leach,chron} \quad \textbf{(183)}$$

$$Clocal_{water,chron} = Clocal_{water,brush}\ Clocal_{water,leach,chron} \quad \textbf{(184)}$$

Input

$Clocal_{water,brush}$	local concentration in water at day one of application	$[kg.d^{-1}]$	O
$Clocal_{soil,brush}$	local emission in soil at the end of day one of application	$[kg.d^{-1}]$	O
$Csoil_{leach,ini}$	concentration of substance in soil due to leaching, for the initial assessment period	$[kg_c.m^{-3}]$	O
$Csoil_{leach,chron}$	concentration of substance in soil due to leaching for the longer assessment period	$[kg_c.m^{-3}]$	O
$Cwater_{leach,ini}$	concentration of substance in water due to leaching, for the initial assessment period	$[kg_c.m^{-3}]$	O
$Cwater_{leach,chron}$	concentration of substance in water due to leaching for the longer assessment period	$[kg_c.m^{-3}]$	O

Output

$Clocal_{water,ini}$	total local concentration in water, initial assessment period	$[kg.d^{-1}]$	O
$Clocal_{soil,ini}$	total local concentration in soil for the initial assessment period	$[kg.d^{-1}]$	O
$Clocal_{water,chron}$	total local concentration in water, chronic assessment period	$[kg.d^{-1}]$	O
$Clocal_{soil,chron}$	total local concentration in soil, chronic assessment period	$[kg.d^{-1}]$	O

III.3.6.6.13 Wood preservatives used in curative and preventive outdoor treatments, injection

Parameters/variables and default values for injection of poles.

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_{ini}$	[d]	30
Temission	$Temission_{chron}$	[d]	>30

Application:

$$Elocal_{soil} = AREA_{pole} \cdot Qprod \cdot Cprod \cdot RHOprod \cdot Fsoil_{inj} \quad \textbf{(185)}$$

$$\mathrm{Clocal}_{\mathrm{soil,inj}} = \frac{\mathrm{Elocal}_{\mathrm{soil,inj}}}{\mathrm{Vsoil} \cdot \mathrm{RHOsoil}} \tag{186}$$

Leaching:

$$Qleach_{ini} = FLUX_{wood,ini} \cdot AREA_{pole} \tag{187}$$

$$Qleach_{chron} = FLUX_{wood,chron} \cdot AREA_{pole} \tag{188}$$

$$Csoil_{leach,.ini} = \frac{Qleach_{ini} \cdot Temission_{ini}}{Vsoil \cdot RHOsoil} \tag{189}$$

$$Csoil_{leach,chron} = \frac{Qleach_{chron} \cdot Temission_{chron}}{Vsoil \cdot RHOsoil} \tag{190}$$

Total concentration:

$$Clocal_{soil,ini} = Clocal_{soil,inj} + Clocal_{soil,leach,ini} \tag{191}$$

$$Clocal_{soil,chron} = Clocal_{soil,inj} + Clocal_{soil,leach,chron} \tag{192}$$

Input			
$AREA_{pole}$	treated wood area during one event	$[m^2]$	D
Q_{prod}	amount of substance used	$[m^3.m^{-2}]$	S
C_{prod}	concentration of active ingredient in used product	[-]	S
RHOprod	density of applied product	$[kg.m^{-3}]$	S
$Fsoil_{inj}$	fraction of product lost to soil during injection	[-]	D
Vsoil	volume of contaminated soil	$[m^3]$	D
RHOsoil	bulk density of wet soil	$[kg.m^{-3}]$	D
$FLUX_{wood,ini}$	average daily flux of the active ingredient over the initial assessment period	$[kg_c.m^{-2}.d^{-1}]$	S
$FLUX_{wood,chron}$	average daily flux of the active ingredient over the chronic assessment period	$[kg_c.m^{-2}.d^{-1}]$	S
$Elocal_{soil,brush}$	local emission to soil during application	[kg]	O
$Clocal_{soil,inj}$	local concentration in soil at the end of day one of application	[kg]	O
$Qleach_{ini}$	average rate of active ingredient leached out of treated wood during the initial assessment period	$[kg_c.d^{-1}]$	O
$Qleach_{chron}$	average rate of active ingredient leached out of treated wood during the chronic assessment period	$[kg_c.d^{-1}]$	O
$Csoil_{leach,ini}$	concentration of substance in soil due to leaching, for the initial assessment period	$[kg_c.m^{-3}]$	O
$Csoil_{leach,chron}$	concentration of substance in soil due to leaching for the longer assessment period	$[kg_c.m^{-3}]$	O
Output			
$Clocal_{soil,ini}$	total local concentration in soil for the initial assessment period	$[kg.kg_{wwrt}^{-1}]$	O
$Clocal_{soil,chron}$	total local concentration in soil, chronic assessment period	$[kg.kg_{wwt}^{-1}]$	O

Table III-77 Default settings for calculating releases from injection

Parameter	Symbol	Unit	Value
Treated wood area	$AREA_{pole}$	[m^2]	0.8
Fraction lost during brushing	$Fsoil_{inj}$	[-]	0.05
Volume of contaminated soil	Vsoil	[m^3]	equation 149
Density of soil	RHOsoil	[$kg_{wwt}.m^{-3}$]	1700

III.3.6.6.14 Wood preservatives used in curative and preventive outdoor treatments, wrapping

Transmission pole:

The calculations of the emission to soil are based on the transmission pole scenario and are therefore not repeated here. The same scenario can be used for this special case, with the remark that only the part below soil has to be considered. The treated wood area (below soil) differs for this scenario. It is set at a value of 0.8 m^2 by default. This scenario is described in section 3.6.20.

Emissions from termite control:

$$\mathrm{Elocal_{air}} = \mathrm{AREA_{ground}} \cdot Qprod \cdot Cprod \cdot RHOprod \cdot F_{air} \qquad \mathbf{(193)}$$

Based on $Qlocal_{soil}$ inputs for soil leaching models can be calculated for predictions of the concentration in ground water.

$$\mathrm{Qlocal_{soil}} = \mathrm{AREA_{ground}} \cdot Qprod \cdot Cprod \cdot RHOprod \cdot (1 - F_{air}) \qquad \mathbf{(194)}$$

Input

$AREA_{ground}$	total area treated per day	[m^2]	D
Q_{prod}	amount of substance used	[$m^3.m^{-2}$]	S
C_{prod}	concentration of active ingredient in used product	[-]	S
$Floss_{air}$	fraction of product emitted to air during application	[-]	D
RHOprod	density of the applied product	[$kg.m^{-3}$]	S
Output			
$Elocal_{air}$	local emission to air during application	[$kg.d^{-1}$]	O
$Qlocal_{soil}$	local quantity applied to soil at day of application	[$kg.d^{-1}$]	O

Table III-78 Default settings for calculating releases from termite control

Parameter	**Symbol**	**Unit**	**Value**
Total treated area	AREAground	[m^2]	287
Fraction lost to air during application	Floss$_{air}$	[-]	
vapour pressure [Pa] at 20 °C:			
< 0.005			0.001
0.005-<0.05			0.01
0.05-<0.5			0.02
0.5-<1.25			0.075
1./25-<2.5			0.15
>2.5			0.25
Density of applied product	RHOprod	[kg.m^{-3}]	-
Application rate of used product	Qprod	[m^3.m^{-2}]	-
Content of active ingredient in product	Cprod	[-]	-

III.3.6.6.15 Concentrations in soil and water taking removal processes into account

Concentrations in soil, taking removal into account:

The following scenarios are used to calculate the time dependent concentration in soil. The situation is based on a single emission event during application, followed by leaching from the treated wood during the service life of the treated product, is considered. This corresponds to the scenarios described in sections 3.6.17 to 3.6.28 for professional and domestic use and service life. The following model could be used to calculate the time dependent concentration for this situation. In case for a given product, in-situ treatment is not applicable, i.e. only pre-treated wood in service is considered, the same model can be used by simply not taking emissions during application into account.

Parameters/variables and default values for calculating the time weighted concentration.

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	Temission$_{ini}$	[d]	30
Temission	Temission$_{chron}$	[d]	>30

$$Clocal_{soil,applic} = \frac{Elocal_{soil,applic}}{Qsoil_{applic}} \quad \textbf{(195)}$$

$$Elocal_{soil,ini} = FLUX_{wood,ini} \cdot AREA_{item} \quad \textbf{(196)}$$

$$Elocal_{soil,chron} = FLUX_{wood,chron} \cdot AREA_{item} \tag{197}$$

$$Clocal_{soil,ini} = \frac{Elocal_{soil,ini}}{Qsoil \cdot k} + \frac{1}{k \cdot Temission_{ini}} \left[Clocal_{soil,appl} - \frac{Elocal_{soil,ini}}{Qsoil \cdot k} \right] \cdot \left(1 - e^{-Temission_{ini} \cdot k}\right)$$

(198)

$$Clocal_{soil,chron} = \frac{Elocal_{soil,chron}}{Qsoil \cdot k} + \frac{1}{k \cdot Temission_{chron}} \left[Clocal_{soil,appl} - \frac{Elocal_{soil,chron}}{Qsoil \cdot k} \right] \cdot \left(1 - e^{-Temission_{chron} \cdot k}\right)$$

(199)

$$Clocal_{soil,pore,ini} = \frac{Clocal_{soil,ini} \cdot RHOsoil}{K_{soil-water}} \tag{200}$$

$$Clocal_{soil,pore,chron} = \frac{Clocal_{soil,chron} \cdot RHOsoil}{K_{soil-water}} \tag{201}$$

Input			
$Qsoil_{applic}$	volume of soil for specific application	$[m^3]$	O
$Elocal_{soil,applic}$	emission to soil during application, over one day	$[kg.d^{-1}]$	O
$Clocal_{soil,appl}$	concentration in soil due to application, for specific scenario	$[kg.d^{-1}]$	O
$Elocal_{soil,ini}$	average daily emission to soil due to leaching over initial assessment period, for specific scenario	$[kg.d^{-1}]$	O
$FLUX_{wood,ini}$	average daily flux of the active ingredient over the initial assessment period	$[kg_c.m^{-2}.d^{-1}]$	S/O
$Elocal_{soil,chron}$	average daily emission to soil due to leaching over the longer assessment period, for specific scenario	$[kg.d^{-1}]$	O
$FLUX_{wood,chron}$	average daily flux of the active ingredient over the chronic assessment period	$[kg_c.m^{-2}.d^{-1}]$	S/O
$AREA_{item}$	leachable wood area for specific item	$[m^2]$	S/O
k	first order rate constant for removal from water	[-]	S
$Clocal_{soil,ini}$	average concentration in soil over initial assessment period, for specific scenario	$[kg.d^{-1}]$	O
$Clocal_{soil,chron}$	average concentration in soil over longer assessment period, for specific scenario	$[kg.d^{-1}]$	O
RHOsoil	bulk density of soil	$[kg.m^{-3}_{soil}]$	O
K_{soil_water}	soil-water equilibrium distribution constant	$[m^3_{soil}.m^{-3}_{water}]$	O^c
Output			
$Clocal_{pore,ini}$	average concentration in pore water over initial assessment period, for specific scenario	$[kg.m^{-3}]$	O
$Clocal_{pore,chron}$	average concentration in pore water over longer assessment period, for specific scenario	$[kg.m^{-3}]$	O

Concentrations in surface water, static water body and flowing water

Two situations can be distinguished: release into a static water body and release into a flowing water body. The first situation corresponds to the scenario for a jetty in a lake (Section 3.6.22). The second situation corresponds to the scenario for a sheet piling (Section

3.6.23) as well as for a wharf on the sea (Section 3.6.24).

In situ-treatment of wooden structures in permanent contact with water is not very likely and therefore only release due to leaching is taken into account.

The following model can be used to take into account removal processes in water bodies.

Parameters/variables and default values for calculating the time weighted concentration in water bodies.

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_{ini}$	[d]	30
Temission	$Temission_{chron}$	[d]	>30

Static water bodies:

$$Elocal_{water,ini} = FLUX_{wood,ini} \cdot AREA_{item} \tag{202}$$

$$Elocal_{water,chron} = FLUX_{wood,chron} \cdot AREA_{item} \tag{203}$$

$$Clocal_{water,ini} = \left(\frac{Elocal_{water,ini}}{Vwater \cdot k} \right) \cdot \left(1 - \frac{1 - e^{-Temission_{ini} \cdot k}}{k \cdot Temission_{ini}} \right) \tag{204}$$

$$Clocal_{water,chron} = \left(\frac{Elocal_{water,chron}}{Vwater \cdot k} \right) \cdot \left(1 - \frac{1 - e^{-Temission_{chron} \cdot k}}{k \cdot Temission_{chron}} \right) \tag{205}$$

To take removal from the water column due to adsorption onto suspended matter into account, the concentration should be calculated as follows:

$$Clocal_{water,diss} = \frac{Clocal_{water,ini}}{(1 + K_{sed-water} \cdot Vsed \cdot Vwater^{-1}) \cdot (1 + Kp_{susp} \cdot SUSP_{water})} \tag{206}$$

$$Clocal_{water,diss} = \frac{Clocal_{water,chron}}{(1 + K_{sed-water} \cdot Vsed \cdot Vwater^{-1}) \cdot (1 + Kp_{susp} \cdot SUSP_{water})} \tag{207}$$

Inpu

Vwater	volume of water for specific scenario	[m^3]	O
$Elocal_{water,ini}$	average daily emission to water due to leaching over initial assessment period, for specific scenario	[$kg.d^{-1}$]	O
$FLUX_{wood,ini}$	average daily flux of the active ingredient over the initial assessment period	[$kg_c.m^{-2}.d^{-1}$]	S/O
$Elocal_{water,chron}$	average daily emission to water due to leaching over the longer assessment period, for specific scenario	[$kg.d^{-1}$]	O
$FLUX_{wood,chron}$	average daily flux of the active ingredient over the chronic assessment period	[$kg_c.m^{-2}.d^{-1}$]	S/O
$AREA_{item}$	leachable wood area for specific item	[m^2]	S/O
k	first order rate constant for removal from water	[-]	S
$Clocal_{water,ini}$	average concentration in water over initial assessment period, for specific scenario	[$kg.d^{-1}$]	O
$Clocal_{water,chron}$	average concentration in water over longer assessment period, for specific scenario	[$kg.d^{-1}$]	O
Vsed	volume of the sediment compartment	[m^3]	D/S
Ksed-water	sediment-water partition coefficient	[$m^3.m^{-3}$]	O
Kp_{susp}	suspended matter-water partition coefficient	[$m^3.kg^{-1}$]	O
$SUSP_{water}$	concentration suspended solids in water body	[$kg.m^{-3}$]	D

Output

$Clocal_{diss,ini}$	average dissolved concentration water over initial assessment period, for specific scenario	[$kg.d^{-1}$]	O
$Clocal_{diss,chron}$	average dissolved concentration in water over longer assessment period, for specific scenario	[$kg.d^{-1}$]	O

Table III-79 Default settings for calculating the concentration in flowing water bodies

Parameter	Symbol	Unit	Value
Volume of the sediment compartment	Vsed	[m^3]	23.56

Flowing water bodies:

Parameters required for distribution modules	Defaults for this scenario	Unit	Value
Temission	$Temission_{ini}$	[d]	30
Temission	$Temission_{chron}$	[d]	>30

$$Elocal_{water,ini} = FLUX_{wood,ini} \cdot AREA_{item} \tag{208}$$

$$Elocal_{water,chron} = FLUX_{wood,chron} \cdot AREA_{item} \tag{209}$$

$$Clocal_{water,ini} = \left(\frac{Elocal_{water,ini}}{Vwater \cdot k}\right) \cdot \left(1 - \frac{1 - e^{-TAU_{wway} \cdot k}}{k \cdot TAU_{wway}}\right) \tag{210}$$

$$Clocal_{water,chron} = \left(\frac{Elocal_{water,chron}}{Vwater \cdot k}\right) \cdot \left(1 - \frac{1 - e^{-TAU_{wway} \cdot k}}{k \cdot TAU_{wway}}\right) \tag{211}$$

To take removal from the water column due to adsorption onto suspended matter into account, the concentration should be calculated as follows:

$$Clocal_{water,diss} = \frac{Clocal_{water,ini}}{(1 + Kp_{susp} \cdot SUSP_{water})} \qquad \textbf{(212)}$$

$$Clocal_{water,diss} = \frac{Clocal_{water,chron}}{(1 + Kp_{susp} \cdot SUSP_{water})} \qquad \textbf{(213)}$$

Inpu			
Vwater	volume of water for specific scenario	$[m^3]$	O
$Elocal_{water,ini}$	average daily emission to water due to leaching over initial assessment period, for specific scenario	$[kg.d^{-1}]$	O
$FLUX_{wood,ini}$	average daily flux of the active ingredient over the initial assessment period	$[kg_c.m^{-2}.d^{-1}]$	S/O
$Elocal_{water,chron}$	average daily emission to water due to leaching over the longer assessment period, for specific scenario	$[kg.d^{-1}]$	O
$FLUX_{wood,chron}$	average daily flux of the active ingredient over the chronic assessment period	$[kg_c.m^{-2}.d^{-1}]$	S/O
$AREA_{item}$	leachable wood area for specific item	$[m^2]$	S/O
k	first order rate constant for removal from water	[-]	S
TAU_{wway}	residence time of water in waterway	[d]	S
$Clocal_{water,ini}$	average concentration in water over initial assessment period, for specific scenario	$[kg.d^{-1}]$	O
$Clocal_{water,chron}$	average concentration in water over longer assessment period, for specific scenario	$[kg.d^{-1}]$	O
Vsed	volume of the sediment compartment	$[m^3]$	D/S
Ksed-water	sediment-water partition coefficient	$[m^3.m^{-3}]$	O
Kp_{susp}	suspended matter-water partition coefficient	$[l_{water}.kg^{-1}{}_{solid}]$	S/O
$SUSP_{water}$	concentration suspended solids in water body	$[l_{solid}.m^{-3}{}_{water}]$	D
Output			
$Clocal_{diss,ini}$	average dissolved concentration water over initial assessment period, for specific scenario	$[kg.d^{-1}]$	O
$Clocal_{diss,chron}$	average dissolved concentration in water over longer assessment period, for specific scenario	$[kg.d^{-1}]$	O

Table III-80 Default settings for calculating the concentration in flowing water bodies

Parameter	**Symbol**	**Unit**	**Value**
Residence time in waterway	TAU_{wway}	[d]	20

III.3.6.7 Product type 9: Fibre, leather, rubber and polymerised materials preservatives

The scenarios and models and equations used in this version of EUSES 2.1.1 for fibre, leather, rubber and polymerised materials preservatives have been taken from the following documents:

- Supplement to the methodology for risk evaluation of biocides Environmental Emission Scenarios for biocides used as Preservatives in rubber and polymerised materials (Product type 9) (European Commission DG ENV / RIVM, 2004).
- Supplement to the methodology for risk evaluation of biocides Environmental Emission Scenarios for biocides used as Preservatives in the leather industry (Product type 9) (Ineris, 2001)
- Supplement to the methodology for risk evaluation of biocides Environmental Emission Scenarios for biocides used as Preservatives in the textile processing industry (Product type 9 & 18) (Ineris, 2001)

These documents can be obtained from the ECB Biocides website

The following modifications are made:
In addition to the original emission scenario methods for estimating the number of emission days has been provided. Also for local plastics production rates the number of emission days have been estimated and tabulated.

III.3.6.7.1 Leather preservatives

<u>Life cycle stage industrial use</u>

Application of biocides at each processing step, curing, pickling, soaking, tanning and finishing:

$$\boldsymbol{Qsubst = Vform \cdot Cform} \qquad \textbf{(214)}$$

$$\boldsymbol{Elocal\_water_i = Qleather \cdot Qsubst_i \cdot (1 - Ffix)} \qquad \textbf{(215)}$$

$$\boldsymbol{Elocal_{3,water} = \sum_{i=1}^{n} Elocal\_water_i} \qquad \textbf{(216)}$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_4$	[d]	220

Input

$Vform_i$	volume of product with preservative applied per kg of paper	$[m^3.kg^{-1}]$	S
$Cform_i$	concentration of active substance in the biocidal product	$[kg_c.m^{-3}]$	S
Qleather	quantity of treated raw hide per day	$[tonnes.d^{-1}]$	D
$Qsubst_i$	quantity of substance used per tonne of leather for treatment step *i*	$[kg_c tonne^{-1}]$	D/P
Ffix	degree of fixation	[-]	S/D
$Elocal\_water_i$	local emission of active substance to water per treatment step	$[kg_c.d^{-1}]$	O
Output			
$Elocal_{3,water}$	total local emission to wastewater	$[kg_c.d^{-1}]$	O

Table III-81 *Defaults for emission calculations.*

Parameter	Symbol	Unit	Value
quantity of treated raw hide per day	Qleather	$[tonne.d^{-1}]$	15
quantity of biocide used per tonne of raw hide	Qsubst	$[kg.tonne^{-1}]$	5¹⁾
degree of fixation	Ffix	[-]	0.95

see pick-list ***Table III-82***

Table III-82 *Pick-list for quantity of biocide used per tonne of leather Qsubst (kg.tonne^{-1}).*

Parameter	Qsubst
curring	0.1-5 (5)
soaking	0.1-5 (5)
pickling	0.1-5 (5)
tanning	0.1-5 (5)
finishing	3

default value presented between brackets

III.3.6.7.2 Textile processing industry, textile preservatives

Life cycle stage industrial use

Desizing and scouring of biocides on imported fabrics

$$Eimport_{3,water} = Qfibres \cdot Cmat \cdot 10^{-9} \qquad (217)$$

Input

Qfibres	quantity of fibres / fabrics per day	$[kg.d^{-1}]$	P
Cmat	estimated content of active substance present in material	$[\mu g_c.kg^{-1}]$	D
Output			
$Eimport_{water}$	local emission to wastewater due to imported material	$[kg_c.d^{-1}]$	O

Table III-83 *Defaults for emission calculations.*

Parameter	**Symbol**	**Unit**	**Value**
quantity of fibres / fabric treated per day	Qfibres	[kg.d^{-1}]	
cotton spinning			7 000
wool preparation			1 000
wool spinning			2 500
silk, synthetic			1 000
sewing knit			4 000
cotton weaving			2 000
wool weaving			1 000
silk weaving			100
others weaving			1 500
textile ennobling			7 000
house and furnish fabric			500
other textile goods			200
cords, filets			3 000
non woven			4 000
mail fabrics			2 000
estimated concentration of active substance present in textile material	Cmat	[μg.kg^{-1}]	
Default			10
Wool			
Default			0.38
DDE			0.07-0.38
PCB-28/31			0.15-0.34
heptachlor			0.03-0.12
Cotton			
Default			12.4
DDE			0.85-4.5
DDD			0.09-12.8
DDT			0-12.4
heptachlor			0.13-0.45

Life cycle stage industrial use

Application of biocides at each textile processing step *(i)*, desizing / scouring, dyeing and finishing (total emissions including emissions due to imported material):

$$Elocal\_water_i = Qfabric \cdot Qsubst_i \cdot (1 - Ffix) \tag{218}$$

$$Elocal_{3,water} = \sum_{i=1}^{n} Elocal\_water_i + Eimport_{water} \tag{219}$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_4$	[d]	225

Input

Qfabric	quantity of treated fabric per day	$[tonnes.d^{-1}]$	D
$Qsubst_i$	quantity of substance used per tonne of fibres/fabric for treatment step *i*	$[kg_c tonne^{-1}]$	S
Ffix	degree of fixation	[-]	S
$Elocal\_water_i$	local emission of active substance to water per treatment step	$[kg_c.d^{-1}]$	O
$Eimport_{water}$	local emission to wastewater due to imported material	$[kg_c.d^{-1}]$	O

Output

$Elocal_{3,water}$	total local emission to wastewater	$[kg_c.d^{-1}]$	O

Table III-84 *Defaults for emission calculations. The highest value is chosen for the worst case situation.*

Parameter	**Symbol**	**Unit**	**Value**
quantity of treated fabric per day	Qfabric	$[tonne.d^{-1}]$	1)
quantity of substance used per tonne of fabric permethrin sulcofuron permethrin/hexahydropyrimidine	Qsubst	$[kg.tonne^{-1}]$	10 0.35-1.81 8-9.7 0.55-0.825
degree of fixation	Ffix	[-]	0.7

1) see Table III-83

2) as a worst case, a default value of 10 kg per tonne can be used if no further data is available

Life cycle stage Service life

$$RELEASEreg_{k,5,water} = \frac{Fprodvol_{reg} \cdot F_{5,water} \cdot Qsubst\_tot_k \cdot \sum_{y=1}^{Tservice_k} (1 - F_{5,j})^{y-1}}{Temission_5} \tag{220}$$

$$RELEASEreg_{5,water} = 10^3 \cdot \sum_{k=1}^{m} RELEASEreg_{k,5,water} \tag{221}$$

$$Elocal_{5,water} = Fmainsource_{5} \cdot RELEASEreg_{5,water} \qquad (222)$$

Input

$Qsubst\_tot_k$	annual input of the substance in article *k*	[tonnes.yr^{-1}]	S
$Fprodvol_{reg}$	fraction of the region	[-]	D
$Tservice_k$	service life of article *k*	[yr]	P
$F_{5,water}$	fraction of the tonnage release over one year during the service to compartment *j*	[-]	S
$Temission_5$	duration of the emission per year	[d.yr^{-1}]	D
$Fmainsource_5$	fraction of the main source (STP)	[-]	D
$RELEASreg_{k,5,water}$	regional release to wastewater for articles *k*	[kg$_c$.d^{-1}]	O
$RELEASreg_{5,water}$	regional release to wastewater for all articles	[kg$_c$.d^{-1}]	O

Output

$Elocal_{5,water}$	local emission to wastewater	[kg$_c$.d^{-1}]	O

Table III-85 Defaults for emission calculations.

Parameter	Symbol	Unit	Value
annual input of the substance in article k	$Qsubst\_tot_k$	[tonnes.yr^{-1}]	.
fraction of the region	$Fprodvol_{reg}$	[-]	0.1
service life of article k	$Tservice_k$	[yr]	[1)]
fraction of the tonnage released over one year during service life	$F_{5,water}$	[-]	.
duration of the emission per year	$Temission_5$	[d.yr^{-1}]	365
fraction of the main source (STP)	$Fmainsource_5$	[-]	0.002

[1)] see pick-list Table III-87

Table III-86 Service life of some article, $Tservice_k$ (yr) some values are averages of the ranges presented in the emission scenario document.

Article	Service life
clothes on contact with skin	1.0
other clothes and bed linen	3.5
household linen	7.5
bedding	5.0
carpets	14.0
wall-to-wall carpet	17.5
sunblind	11.5
tents	12.5
awning	2.0

III.3.6.7.3 Preservatives used in rubber materials

For biocides applied in rubber products, use emission scenario document on IC 11 Rubber industry, thought no specific data for biocides is reported.

III.3.6.7.4 Paper industry, fibre preservatives

The specific scenario is described under product type 7, see section III.3.6.10.

III.3.6.7.5 Preservatives used in polymerised materials

The emission scenario for the release of biocides from manufacture of plastic materials, service life and waste treatment of polymers is based on the OECD emission scenario document on plastics additives (OECD, 2004).

Industrial use

This section deals with the emission scenario for the release of biocides from manufacture of plastic materials (handling, compounding, and conversion).

This emission scenario for handling is only applicable to solid materials (powders). Emission factors for liquids are not available yet.
As a worst case all the emissions are assumed to waste water. Waste stage is considered not to be relevant because waste should be treated as chemical waste, which is not landfilled.
For emission estimation, the particle size distribution of the handled substance has to be submitted by the applicant.

Handling

$$Fhandl_{water} = Fhandl_{water,<40\,\mu m} \cdot Fpart_{<40\mu m} + Fhandl_{water,>40\,\mu m} \cdot Fpart_{>40\mu m} \tag{223}$$

Compounding

$$Fcomp_{air} = 0.5 \cdot Fcomp_{volat} \tag{224}$$

$$Fcomp_{water} = Fcomp_{water,<40\,\mu m} \cdot Fpart_{<40\mu m} + Fcomp_{water,>40\,\mu m} \cdot Fpart_{>40\mu m} + 0.5 \cdot Fcomp_{volat}$$

Conversion

(225)

Inorganic substances

$$Fconv_{water} = Fconv\_water \tag{226}$$

Organic substances

$$Fconv_{air} = Fconv_{water} = 0.5 \cdot Fconv_{volat} \tag{227}$$

Overall

$$F_{3,.air} = Fhandl_{air} + Fcomp_{air} + Fconv_{air} \tag{228}$$

$$F_{3,.water} = Fhandl_{water} + Fcomp_{water} + Fconv_{water} \qquad \textbf{(229)}$$

The emission scenario does not provide the number of emission days. To establish the number of emission days and size of a point source for emission estimation at the local scale table B3.9 for industrial category 11, of Appendix I of the Technical Guidance Document (EC, 2003) should be used to calculate the number of emission days (Temission). The regional tonnage, TONNAGEreg, should be corrected for the estimation of the fraction of the main source and the number of emission days by the concentration or fraction of the substance in the polymer (Fpolymer). This yields the tonnage of the polymer in the EU. The concentration in the polymer has to be supplied by the notifier. The fraction of the tonnage for the region is by default 0.1 for existing substance with wide spread use. For new substances with limited use the fraction of the tonnage for the region is by default 1, according to the TGD (EC, 2003).

$$TONNAGEreg = Fprodvolreg \cdot TONNAGE \qquad \textbf{(230)}$$

$$TONNAGEreg_{polymer} = TONNAGEreg / Fpolymer \qquad \textbf{(231)}$$

$$Elocal_{3,air} = TONNAGEreg \cdot Fmainsource_3 \cdot F_{3,air} \cdot \frac{365}{Temission_3} \qquad \textbf{(232)}$$

$$Elocal_{3,water} = TONNAGEreg \cdot Fmainsource_3 \cdot F_{3,water} \cdot \frac{365}{Temission_3} \qquad \textbf{(233)}$$

Alternatively local production rates (Qplastic) for different types of polymers and for each processing type can be used (***Table III-91***). The production rates provided in the emission scenario specifically refer to the situation in the United Kingdom. Therefore using these data should be done with care as the distribution of size of companies may differ might differ from one country to another. Using the local production rates the number of working days can be estimated from the information provided in Table B3.9 from the TGD. The number of working days is listed in ***Table III-92***).

$$Elocal_{3,air} = Qplastic \cdot Fpolymer \cdot F_{3,air} /Nwdays \qquad \textbf{(234)}$$

$$Elocal_{3,water} = Qplastic \cdot Fpolymer \cdot F_{3,water} /Nwdays \qquad \textbf{(235)}$$

Input

-	processing system	[-]	P
-	polymer type	[-]	P
-	type of substance	[-]	P
-	type of conversion process	[-]	P
-	type of product	[-]	P
VOLATILITY	volatility of the substance	[High/medium/low]	S
WATERRINSE	Is water used for cleaning operations?	[yes/no]	P
Fpart$_{<40\ \mu m}$	particle size fraction < 40 um	[-]	S
Fpart$_{>40\ \mu m}$	particle size fraction > 40 um	[-]	S
Fhandl$_{water,<40\ \mu m}$	fraction released to water for particle size fraction < 40 µm	[-]	D
Fhandl$_{water,>40\ \mu m}$	fraction released to water for particle size fraction > 40 µm	[-]	D
Fhandl$_{air,<40\ \mu m}$	fraction released to air for particle size fraction < 40 µm	[-]	D
Fhandl$_{air,>40\ \mu m}$	fraction released to air for particle size fraction > 40 µm	[-]	D
Fcomp$_{water,<40\ \mu m}$	fraction released to water for particle size fraction < 40 µm	[-]	S
Fcomp$_{water,>40\ \mu m}$	fraction released to water for particle size fraction > 40 µm	[-]	S
Fhandl$_{air}$	fraction released to air during materials handling	[-]	O^c
Fhandl$_{water}$	fraction released to water during materials handling	[-]	O^c
Fcomp$_{volat}$	fraction released at compounding, which is related to the volatility of the substance used	[-]	D
Fcomp$_{air}$	fraction release to air during compounding	[kg.kg^{-1}]	O^c
Fcomp$_{water}$	fraction release to water during compounding	[kg.kg^{-1}]	O^c
Fconv$_{volat}$	fraction released at conversion, which is related to the volatility of the substance used	[-]	D
Fcomp$_{air}$	fraction release to air during compounding	[kg.kg^{-1}]	O^c
Fcomp$_{water}$	fraction release to water during compounding	[kg.kg^{-1}]	O^c
F3,air	emission factor to air for processing	[-]	O
F3,water	emission factor to (waste)water for processing	[-]	O
TONNAGE	relevant tonnage of the substance in EU for this application	[kg.d^{-1}]	S
TONNAGEreg	relevant tonnage the substance in the region for this application	[kg.d^{-1}]	S/O
Fpolymer	fraction of active substance in the in the plastic material	[kg.kg^{-1}]	S
Fprodvol$_{reg}$	fraction for the region	[-]	D
TONNAGEreg$_{polymer}$	amount of plastic produced with the substance in the region	[kg.d^{-1}]	O
Fmainsource$_3$	fraction of the main source for polymer processing	[-]	D
Temission$_3$	number of emission days	[d]	O
Nwdays	number of working days at the local source	[d.yr^{-1}]	D/O
Qplastic	local production rate for specific type of plastic and process	[kg.yr^{-1}]	D/O

Output

Elocal$_{3,water}$	local emission of active substance to waste water	[kg$_c$.d^{-1}]	O
Elocal$_{3,air}$	local emission of active substance to waste water	[kg$_c$.d^{-1}]	O

Table III-87 Default settings for calculating releases of biocides used as preservatives in the polymers industry

Parameter	**Symbol**	**Unit**	**Value**
Quantity of plastic produced	Qplastic	[kg.d^{-1}]	***Table III-91***
Fraction released to water during materials handling	Fhandling$_{water}$	[-]	
WATERRINSE = no			n.a.*
WATERRINSE = yes			
particle size < 40 um			0.006
particle size > 40 um			0.002
Fraction volatilised during compounding**	Fcomp$_{volat}$	[-]	
Volatility at: 20 C° 150 C°:			
high > 1.10^{-4} Pa > 50 Pa			0.0005
medium 1.10^{-4} – 1.10^{-5} Pa 5-50 Pa			0.0001
low < 1.10^{-5} Pa < 5 Pa			0.00002
Fraction released to water during compounding	Fcomp$_{water}$	[-]	
WATERRINSE = no			n.a.*
WATERRINSE = yes			
particle size < 40 um			0.0005
particle size > 40 um			0.0001
Fraction released to water during conversion	Fconv_water	[-]	
Inorganic substances			
Conversion process			
- grinding/machining			0.025
- other processes			0.0001
Organic substance			n.a.
Fraction of substance volatilised during conversion	Fconv$_{volat}$	[-]	
Inorganic substances			n.a.
Organic substance			***Table III-88***

n.a.: not applicable.

* Waste generated from the processing stages is considered not applicable because it should be treated as chemical waste and as such not be released at landfills.

** if processing temperature (compounding or conversion) is exceeding 200 °C then emission factor should by a factor of ten higher

Table III-88 Default emission factors, $Fconv_{volat}$ (-) for different conversion processes and types of articles produced based on the vapour pressure (Pa) at 150 C° of the applied substance. High (> 50 Pa), medium (5 - 50 Pa) and low (<5 Pa) vapour pressure.

Type of Process	Type of product	Vapour pressure	Value*
Open	solid		
		high	0.0025
		medium	0.0005
		low	0.0001
	foamed	high	0.005
		medium	0.001
		low	0.0002
Partially open	All	high	0.0015
		medium	0.0003
		low	0.00006
Closed	All	high	0.0005
		medium	0.0001
		low	0.00002

* if processing temperature (compounding or conversion) is exceeding 200 °C then emission factor should by a factor of ten higher

Table III-89 Default settings for calculating concentrations in the STP or surface water and air of compounds used in polymers

Parameter	Symbol	Unit	Value
Fraction for the region	$Fprodvol_{reg}$	[-]	0.1

Table III-90 Fraction of the main source, $Fmainsource_3$ [-], and the number of emission days, Temission3 [d], for the processing stage of polymers and polymers with preservatives based on the corrected regional tonnage, $TONNAGEreg_{polymer}$ [tonnes .yr^{-1}], of the biocide

$TONNAGEreg_{polymer}$	$Fmainsource_3$	$Temission_3$
< 10	0,5	2 · Fmainsource · TONNAGEreg
≥10-<50	0,35	Fmainsource · TONNAGEreg
≥50-<500	0.25	0.4 · Fmainsource · TONNAGEreg
≥500-<5,000	0.15	0.4 · Fmainsource · TONNAGEreg
≥5,000-<25,000	0.10	300
≥ 25,000	0.05	300

Table III-91 Local production rates, Qplastic (kg.yr^{-1}) for different types of polymers

Polymer type	**Local production rate**		
	open	**partially open**	**closed**
Low density polyethylene (LDPE)		23 100 000	528 000
High density polyethylene (HDPE)		2 070 000	2 130 000
Polypropylene (PP)		8 880 000	1 610 000
Rigid Polyvinylchloride (R-PVC)	988 000		2 010 000
Flexible Polyvinylchloride (F-PVC)	744 000	3 990 000	341 000
Polystyrene (PS)	605 000	389 000	623 000
Expanded Polystyrene (EPS)			2 790 000
Acrylonitrile-Butadiene-Styrene (ABS)	78 000		428 000
Polyethylene terephtalate (PET)	176 000		814 000
Polyamides (PA)	39 000		181 000
Acrylics (AL)	55 000	207 000	28 000
Acetals (AT)		52 000	84 000
Polycarbonates (PC)		62 000	69 000
Polyurethanes (PU)			804 000
Unsaturated polyesters (UP)	575 000		206 000
Phenolic resins (PR)			121 000
Amino resins (AR)			469 000
Epoxy resins (ER)			80 000

Table III-92 Local number of production days, Nwdays (d.yr^{-1}) for different types of polymers

Polymer type	**Local production rate**		
	open	**partially open**	**closed**
Low density polyethylene (LDPE)		300	300
High density polyethylene (HDPE)		300	300
Polypropylene (PP)		300	300
Rigid Polyvinylchloride (R-PVC)	300		300
Flexible Polyvinylchloride (F-PVC)	298	300	136
Polystyrene (PS)	242	156	249
Expanded Polystyrene (EPS)			300
Acrylonitrile-Butadiene-Styrene (ABS)	31		171
Polyethylene terephtalate (PET)	70		300

Polyamides (PA)	16		72
Acrylics (AL)	22	83	11
Acetals (AT)		21	34
Polycarbonates (PC)		25	28
Polyurethanes (PU)			300
Unsaturated polyesters (UP)	230		82
Phenolic resins (PR)			48
Amino resins (AR)			188
Epoxy resins (ER)			32

Release during service life

As a worst case it is assumed that all release due to leaching and abrasion is to waste water for both outdoor and indoor applications.

$$Qsubst\_tot_k = Qplastic\_tot_k \cdot Fpolymer_k \cdot Fpenetr_k \tag{236}$$

Emission factors

For organic compounds:

Water

if Tservice$_k$ = < 4, then Tservice$_k$ – 4 = 0

$$Foutdoor_{service,water,k} = Forg\_T4_{service,water} \frac{Tservice_k}{4} + Forg\_T > 4_{service,water} \cdot (Tservice_k - 4) \tag{237}$$

if Tservice$_k$ = > 4, then

$$Foutdoor_{service,water,k} = Forg\_T4_{service,water} + Forg\_T > 4_{service,water} \cdot (Tservice_k - 4)$$

Surface water

$$F_{service,water,k} = Foutdoor_{service,water,k} \cdot Fuse_{outdoor,k} \tag{238}$$

Waste water (Regional STP)

$$F_{service,water,k} = Findoor_{service,water} \cdot (1 - Fuse_{outdoor,k}) \tag{239}$$

For inorganic compounds

Surface water

$$F_{service,water,k} = F_{service,water,k} \cdot Fuse_{outdoor,k} \tag{240}$$

Waste water (Regional STP)

$$F_{service,wastewater,k} = F_{service,water} \cdot (1 - Fuse_{outdoor,k}) \tag{241}$$

General calculations of the release/emission of organic compounds and inorganic compounds to air, waste water (indoor) and surface water (outdoor):

$$RELEASEreg_{k,service,j} = Fprodvol_{reg} \cdot F_{service,j,k} \cdot Qsubst\_tot_{k} \cdot \frac{1}{Temission_{service}} \tag{242}$$

$$RELEASEreg_{service,j} = \sum_{k=1}^{m} RELEASEreg_{k,service,j} \tag{243}$$

$$Elocal_{service,wastewater} = Fmainsource_{service} \cdot RELEASEreg_{service,wastewater} \tag{244}$$

Input			
$Qsubst\_tot_{k}$	annual input of the substance in article *k*	[kg.yr^{-1}]	S/O
$Qplastic\_tot_{k}$	annual input of plastic article *k*	[kg.yr^{-1}]	S
$Fpolymer_{k}$	fraction of active substance in plastic article *k*	[kg$_{c}$.kg^{-1}]	S
$Fpenetr_{k}$	penetration rate of substance in plastic article *k*	[-]	D/S
$Qsubst\_acc_{k}$	total accumulated amount of the substance in article *k* (per year) at steady state	[kg$_{c}$]	S
$Fprodvol_{reg}$	fraction of the region	[-]	D
-	type of application for plastic article	[-]	P
$Tservice_{k}$	service life of article *k*	[yr]	O
$Temission_{service}$	number of emission days per year	[d.yr^{-1}]	D
-	type of substance	[-]	P
$Forg\text{-}T4_{service,water}$	fraction released to water during service life in first 4 years of product life	[-]	D
$Forg\text{-}T{>}4_{servic,water}$	fraction released to water per year during service life in period after first four years of service life	[-]	D
$Fused_{outdoor,k}$	fraction of amount of article with outdoor application	[-]	D
$Foutdoor_{service,water,k}$	fraction of substance released per year during the whole service life to (waste) water for article *k*	[-]	D
$F_{service,j,k}$	fraction of substance released per year during the whole service life from article *k* to compartment *j*	[-]	D
$Fmainsource_{service}$	fraction of the main source	[-]	D
Output			
$RELEASEreg_{k,service,j}$	regional release for the stage of service life to compartment *j* for product *k*	[kg.d^{-1}]	O
$RELEASEreg_{service,j}$	total regional release for the stage of service life to compartment *j* for all *m* products with the biocide	[kg.d^{-1}]	O
$Elocal_{service,wastewater}$	total local emission to waste water for the stage of service life to wastewater from all products	[kg.d^{-1}]	O

Table III-93 Default settings for the input parameters of the model for calculating the releases from plastic articles during their service life

Parameter	**Symbol**	**Unit**	**Value**
Fraction of mass released during service life	$F_{service,j}$	[-]	
Inorganic compounds			
air			0
waste water			0.0001
Organic compounds			
air			0.0005
(waste) water			
indoor			0.0005
outdoor			Equation 240
Fraction released to water during service life in first 4 years of product life	Forg_T4	[-]	0.007
Fraction released to water per year during service life in period after first four years of service life	Forg_T>4	[-]	0.0015
Fraction of amount of article with outdoor application	$Foutdoor_k$	[-]	***Table III-94***
Penetration rate of the substance in article k	$Fpenetr_k$	[-]	1
Fraction of the region	$Fprodvol_{reg}$	[-]	0.1
Fraction of the mainsource$_{service}$	$Fmainsoure_{service}$	[-]	0.002
Number of emission days per year	$Temission_{service}$	[$d.yr^{-1}$]	365

Table III-94 Default settings for Service life, Tservicek (yr) and the fraction used in outdoor applications, $Fuse_{outdoor}$ (-) of article k for different means of use.

Application	**$Tservice_k$**	**$Foutdoor_k$**
agricultural application	2	1
building and construction	10	0.5
white goods	5	0
brown goods	5	0
electrical	10	0
electronic	1	0
furniture	5	0.5
house wares	1	0
marine	10	1
packaging	2	0.5
sports	1	0.5
transport and automotive	10	1
miscellaneous	1	0.5

III.3.6.7.6 Preservatives used in rubber materials

This type of use actually applies to the emission scenario for industrial category IC-11, polymers industry. As part of this IC, the rubber industry (formerly IC 15/0 others) can be identified. There is no specific information which relates to the use of biocides in this industrial category.

III.3.6.8 Product type 10: Masonry preservatives

The scenarios and models and calculation formulations used in this version of EUSES 2.1.1 for masonry preservatives have been taken from the following documents:

- Supplement to the methodology for risk evaluation of biocides Environmental Emission Scenarios for biocides used as masonry preservatives (Product type 10) (Ineris, 2002)

This document can be obtained from the ECB Biocides website

Industrial use

Industrial sites

There is usually no treatment at industrial sites. Generally biocides are not use at the production of cement, extraction and processing of clay or added to concrete. It is assumed that neither biocides are used to treat products after production and before being marketed.

Private and professional use

In situ treatment of buildings (preventive and curative)

Surfaces made of building materials such as roofs, walls, façades, paths, terraces, etc. can be affected by the development of mosses, lichen, and algae. Biocides can be used to protect and/ or cure building materials.

III.3.6.8.1 Masonry preservatives used at situ treatment, spraying

Parameters/variables and default values for a roof treated through spraying.

Countryside

if GUTTER = no, then

$$Elocal\_soil_{spray-drift,roof} = AREAroof \cdot Vform \cdot Fform \cdot RHOform \cdot Fdrift \qquad \textbf{(245)}$$

$$Elocal\_soil_{runoff,roof} = AREAroof \cdot Vform \cdot Fform \cdot RHOform \cdot Frunoff \qquad \textbf{(246)}$$

$$Csoil\_adjacent_{roof} = \frac{Elocal\_soil_{runoff,roof}}{Vsoil\_adjacent \cdot RHOsoil} \qquad \textbf{(247)}$$

$$Csoil\_distant_{roof} = \frac{Elocal\_soil_{spray-drift,roof}}{Vsoil\_distant \cdot RHOsoil} \qquad \textbf{(248)}$$

if GUTTER = yes, then

$$Elocal\_water_{roof} = \frac{AREAroof \cdot Vform \cdot Fform \cdot RHOform \cdot Frunoff}{Temission_{spray}} \qquad \textbf{(249)}$$

$$Csoil\_distant_{roof} = \frac{Elocal\_soil_{spray-drift,roof}}{Vsoil\_distant \cdot RHOsoil} \qquad \textbf{(250)}$$

City

$$Elocal\_water_{roof} = \frac{AREAroof \cdot Vform \cdot Fform \cdot RHOform \cdot (Frunoff + Fdrift)}{Temission_{spray}} \qquad \textbf{(251)}$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_{spary}$	[d]	1

Input			
GUTTER	roof fitted with a gutter	[yes/no]	P
AREAroof	roof area treated per day	[m^2]	D
Vform	fluid application rate of applied formulation	[$m^3.m^{-2}$]	S
RHOproduct	density of product	[$kg.m^{-3}$]	S/D
Fform	fraction of active ingredient in applied formulation	[$kg_c.kg$]	S
Fdrift	fraction of product lost during application due to spray drift	[-]	D
Frunoff	fraction of product lost during application due to runoff	[-]	D
$Vsoil\text{-}adjacent_{roof}$	volume of soil adjacent to treated roof	[m^3]	D
$Vsoil\text{-}distant_{roof}$	volume of soil distant to treated roof	[m^3]	D
RHOsoil	bulk density of wet soil	[$kg_{wwt}.m^3$]	D
$Temission_{spray}$	number of emission days for spraying	[d]	D
$Elocal\ \_soil_{spray\text{-}drift,roof}$	local emission to soil from spray-drift, distant to roof	[kg_c]	O^c
$Elocal\_soil_{runoff,roof}$	local emission to soil from runoff, adjacent to roof	[kg_c]	O^c
Output			
$Elocal\_water_{roof}$	local emission to waste water during episode	[$kg_c.d^{-1}$]	O
$Csoil\text{-}adjacent_{roof}$	local concentration in soil adjacent to roof	[$kg_c.kg_{wwt}^{-1}$]	O
$Csoil\text{-}distant_{roof}$	local concentration in soil distant to roof	[$kg_c.kg_{wwt}^{-1}$]	O
Temission	number of emission days	[d]	O

Table III-95 Default settings for roof spraying.

Parameter	**Symbol**	**Unit**	**Value**
Roof fitted with gutter	GUTTER	[yes/no]	no
Roof area treated per day	AREAroof	[m^2]	145
Fluid application rate of product	Vform	[$m^3.m^{-2}$]	-
Fraction of active ingredient in product	Fform	[$kg_c.kg$]	-
Density of product	RHOform	[$kg.m^{-3}$]	1000
Fraction of product lost by spray drift	Fdrift	[-]	0.1
Fraction of product lost due to runoff	Frunoff	[-]	0.2
Volume of soil adjacent to roof	$Vsoil\text{-}adjacent_{roof}$	[m^3]	0.5
Volume of soil distant to roof	$Vsoil\text{-}distant_{roof}$	[m^3]	54.1
Bulk density of wet soil	RHOsoil	[$kg_{wwt}.m^{-3}$]	1700
Number of emission days for spraying	$Temission_{spray}$	[d]	1

Parameters/variables and default values for a façade treated by spraying.

Countryside

$$Elocal\_soil_{spray-drift,\,façade} = AREA_{façade} \cdot Vform \cdot Fform \cdot RHOform \cdot Fdrift \tag{252}$$

$$Elocal\_soil_{runoff,\,façade} = AREA_{façade} \cdot Vform \cdot Fform \cdot RHOform \cdot Frunoff \tag{253}$$

$$Csoil\_adjacent_{façade} = \frac{Elocal\_soil_{runoff,\,façade}}{Vsoil\_adjacent \cdot RHOsoil} \tag{254}$$

$$Csoil\_distant_{façade} = \frac{Elocal\_soil_{spray-drift,\,façade}}{Vsoil\_distant \cdot RHOsoil} \tag{255}$$

City

$$Elocal\_water_{façade} = \frac{AREAfaçade \cdot Vform \cdot Fform \cdot RHOform \cdot (Frunoff + Fdrift)}{Temission_{spray}} \tag{256}$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_{spary}$	[d]	1

Input			
COMB	Simultaneous treatment of roof and façade	[yes/no]	P
AREAfaçade	façade area treated per day	[m^2]	D
Vform	fluid application rate of applied formulation	[$m^3.m^{-2}$]	S
RHOproduct	density of formulation	[$kg.m^{-3}$]	S/D
Fform	fraction of active ingredient in formulation	[$kg_c.kg$]	S
Fdrift	fraction of product lost during application due to spray drift	[-]	D
Frunoff	fraction of product lost during application due to runoff	[-]	D
$Vsoil\text{-}adjacent_{façade}$	volume of soil adjacent to treated object	[m^3]	D
$Vsoil\text{-}distant_{façade}$	volume of soil distant to treated object	[m^3]	D
RHOsoil	bulk density of wet soil	[$kg_{wwt}.m^3$]	D
$Temission_{spray}$	number of emission days for spraying	[d]	D
$Elocal\ \_soil_{spray\text{-}drift,façade}$	local emission to soil from spray-drift, distant to façade	[kg_c]	O^c
$Elocal\_soil_{runoff,façade}$	local emission to soil from runoff, adjacent to façade	[kg_c]	O^c
Output			
$Elocal\_water_{façade}$	local emission to waste water during episode	[$kg_c.d^{-1}$]	O
$Csoil\text{-}adjacent_{façade}$	local concentration in soil adjacent to façade	[$kg_c.kg_{wwt}^{-1}$]	O
$Csoil\text{-}distant_{façade}$	local concentration in soil distant to façade	[$kg_c.kg_{wwt}^{-1}$]	O
Temission	number of emission days	[d]	O

Table III-96 Default settings for façade spraying.

Parameter	**Symbol**	**Unit**	**Value**
Simultaneous treatment of roof and façade	COMB	[yes/no]	yes
Area of façade treated per day	AREAfaçade	[m^2]	125
Fluid application rate of product	Vform	[$m^3.m^{-2}$]	-
Fraction of active ingredient in product	Fform	[$kg_c.kg$]	-
Density of product	RHOform	[$kg.m^{-3}$]	1000
Fraction of product lost by spray drift	Fdrift	[-]	0.1
Fraction of product lost due to runoff	Frunoff	[-]	0.2
Volume of soil adjacent to façade	$Vsoil\text{-}adjacent_{façade}$	[m^3]	0.5
Volume of soil distant to façade COMB = yes COMB = no	$Vsoil\text{-}distant_{façade}$	[m^3]	 54.1 27.3
Bulk density of wet soil	RHOsoil	[$kg_{wwt}.m^{-3}$]	1700
Number of emission days for spraying	$Temission_{spray}$	[d]	1

Parameters/variables and default values for a combined treatment of the roof and façade through spraying.

if COMB = yes and GUTTER = no, then

Countryside

$$Csoil\_adjacent = Csoil\_adjacent_{\mathrm{roof}} + Csoil\_adjacent_{façade} \qquad \textbf{(257)}$$

$$Csoil\_distant = Csoil\_distant_{\mathrm{roof}} + Csoil\_distant_{façade} \qquad \textbf{(258)}$$

if COMB = yes and GUTTER = yes, then

$$Elocal_{3,water} = Elocal\_water_{\mathrm{roof}} \qquad \textbf{(259)}$$

$$Csoil\_adjacent = Csoil\_adjacent_{façade} \qquad \textbf{(260)}$$

$$Csoil\_distant = Csoil\_distant_{\mathrm{roof}} + Csoil\_distant_{façade} \qquad \textbf{(261)}$$

City

$$Elocal_{3,water} = Elocal\_water_{\mathrm{roof}} + Elocal\_water_{façade} \qquad \textbf{(262)}$$

Input			
Csoil-adjacent$_{roof}$	local concentration in soil adjacent to roof	[$kg_c.kg_{wwt}^{-1}$]	O
Csoil-distant$_{roof}$	local concentration in soil distant to roof	[$kg_c.kg_{wwt}^{-1}$]	O
Csoil-adjacent$_{façade}$	local concentration in soil adjacent to façade	[$kg_c.kg_{wwt}^{-1}$]	O
Csoil-distantf$_{açade}$	local concentration in soil distant to façade	[$kg_c.kg_{wwt}^{-1}$]	O
Elocal_water$_{roof}$	local emission to waste water from roof treatment	[$kg_c.d^{-1}$]	O
Elocal_water$_{façade}$	local emission to waste water from façade treatment	[$kg_c.d^{-1}$]	O
Output			
Csoil_adjacent	local concentration in soil adjacent to house	[$kg_c.kg_{wwt}^{-1}$]	O
Csoil_distant	local concentration in soil adjacent to house	[$kg_c.kg_{wwt}^{-1}$]	O
Elocal$_{3,water}$	emission to waste water	[$kg_c.d^{-1}$]	O

III.3.6.8.2 Masonry preservatives used for situ treatment, rolling and brushing

Parameters/variables and default values for a roof treated by brushing or rolling.

Countryside

$$Elocal\_soil_{roof} = AREAroof \cdot Vform \cdot Fform \cdot RHOform \cdot Fdripping \tag{263}$$

$$Csoil\_adjacent_{roof} = \frac{Elocal\_soil_{roof}}{Vsoil\_adjacent \cdot RHOsoil} \tag{264}$$

City

$$Elocal\_water_{roof} = \frac{AREAroof \cdot Vform \cdot Fform \cdot RHOform \cdot Fdripping}{Temission_{roll}} \tag{265}$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	Temission$_{roll}$	[d]	1

Input			
AREAroof	roof area treated per day	[m^{2}]	D
Vform	fluid application rate of applied formulation	[m^{3}.m^{-2}]	S
RHOproduct	density of product	[kg.m^{-3}]	S/D
Fform	fraction of active ingredient in formulation	[kg$_{c}$.kg]	S
Fdripping	fraction of product lost during application due to dripping	[-]	D
Vsoil-adjacent$_{roof}$	volume of soil adjacent to treated object	[m^{3}]	D
RHOsoil	bulk density of wet soil	[kg$_{wwt}$.m^{3}]	D
Temission$_{roll}$	number of emission days for rolling	[d]	D
Output			
Elocal _soil$_{roof}$	local emission to soil from spray-drift, distant to roof	[kg$_{c}$]	O
Elocal_water$_{roof}$	local emission to waste water from roof treatment	[kg$_{c}$.d^{-1}]	O
Csoil-adjacent$_{roof}$	local concentration in soil adjacent to roof	[kg$_{c}$.kg$_{wwt}$$^{-1}$]	O
Temission	number of emission days	[d]	O

Table III-97 Default settings for roof treatment by brushing or rolling.

Parameter	**Symbol**	**Unit**	**Value**
Roof area treated per day	AREAroof	[m^2]	145
Fluid application rate of product	Vform	[m^3.m^{-2}]	-
Fraction of active ingredient in product	Fform	[-]	-
Density of product	RHOform	[kg.m^{-3}]	1000
Fraction of product lost due to dripping	Fdripping	[-]	
Professional use			0.03
Amateur use			0.05
Volume of soil adjacent to roof	Vsoil-adjacent$_{roof}$	[m^3]	0.5
Bulk density of wet soil	RHOsoil	[kg.m^{-3}]	1700
Number of emission days for rolling and brushing	Temission$_{roll}$	[d]	1

Parameters/variables and default values for a façade treated through rolling or brushing.

Countryside

$$Elocal\_soil_{façade} = AREAfaçade \cdot Vform \cdot Fform \cdot RHOform \cdot Fdripping \tag{266}$$

$$Csoil\_adjacent_{façade} = \frac{Elocal\_soil_{façade}}{Vsoil\_adjacent \cdot RHOsoil} \tag{267}$$

City

$$Elocal\_water_{façade} = \frac{AREAfaçade \cdot Vform \cdot Fform \cdot RHOform \cdot Fdripping}{Temission_{roll}} \tag{268}$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	Temission$_{roll}$	[d]	1

Input			
AREAfaçade	façade area treated per day	[m^2]	D
Vform	fluid application rate of applied formulation	[m^3.m^{-2}]	S
RHOproduct	density of product	[kg.m^{-3}]	S/D
Fform	fraction of active ingredient in formulation	[kg$_c$.kg]	S
Fdripping	fraction of product lost during application through dripping	[-]	S
Vsoil-adjacent$_{\text{façade}}$	volume of soil adjacent to treated object	[m^3]	D
RHOsoil	bulk density of wet soil	[kg$_{wwt}$.m^3]	D
Temission$_{\text{roll}}$	number of emission days for rolling and brushing	[d]	D
Output			
Elocal _soil$_{\text{façade}}$	local emission to soil from spray-drift, distant to façade	[kg$_c$]	O
Elocal_water$_{\text{façade}}$	local emission to waste water during episode	[kg$_c$.d^{-1}]	O
Csoil-adjacent$_{\text{façade}}$	local concentration in soil adjacent to façade	[kg$_c$.kg$_{wwt}$$^{-1}$]	O
Temission	number of emission days	[d]	O

Table III-98 Default settings for façade treatment by rolling or brushing.

Parameter	**Symbol**	**Unit**	**Value**
Area of façade treated per day	AREAfaçade	[m^2]	125
Fluid application rate of product	Vform	[m^3.m^{-2}]	-
Fraction of active ingredient in product	Fform	[kg$_c$.kg]	-
Density of product	RHOform	[kg.m^{-3}]	1000
Fraction of product lost due to dripping	Fdripping	[-]	
Professional use			0.03
Amateur use			0.05
Volume of soil adjacent to façade	Vsoil-adjacent$_{\text{façade}}$	[m^3]	0.5
Bulk density of wet soil	RHOsoil	[kg$_{wwt}$.m^{-3}]	1700
Number of emission days for brushing or rolling	Temission$_{\text{roll}}$	[d]	1

Parameters/variables and default values for a combined treatment of the roof and façade through brushing or rolling.

if COMB = yes, then

Countryside

$$Csoil\_adjacent = Csoil\_adjacent_{\mathrm{roof}} + Csoil\_adjacent_{fa\text{çade}} \tag{269}$$

City

$$Elocal_{3,water} = Elocal\_water_{\mathrm{roof}} + Elocal\_water_{fa\text{çade}} \tag{270}$$

Input			
Csoil-adjacent$_{roof}$	local concentration in soil adjacent to roof	[kg$_c$.kg^{-1}]	O
Csoil-adjacent$_{façade}$	local concentration in soil adjacent to façade	[kg$_c$.kg^{-1}]	O
Elocal_water$_{roof}$	local emission to waste water from roof treatment	[kg$_c$.d^{-1}]	O
Elocal_water$_{façade}$	local emission to waste water from façade treatment	[kg$_c$.d^{-1}]	O
Output			
Csoil_adjacent	local concentration in soil adjacent to house	[kg$_c$.kg^{-1}]	O
Elocal$_{3,water}$	emission to waste water	[kg$_c$.d^{-1}]	O

Table III-99 Default settings for combined treatment of roof and façade by rolling or brushing.

Parameter	Symbol	Unit	Value
Simultaneous treatment of roof and facade	COMB	[yes/no]	yes

III.3.6.8.3 Masonry preservatives used for in- situ treatment, rinse

Parameters/variables and default values for release during rinse with high pressure spraying.

Release depends on the way of application to the substrate (*i*), either spraying or rolling and brushing. Relevant stage of the life cycle is waste treatment, stage 7.

$$Frinse_{spray} = 1 - Fdrift - Frunoff - Felim \qquad \mathbf{(271)}$$

$$Frinse_{roll} = 1 - Fdripping - Felim \qquad \mathbf{(272)}$$

Countryside

if GUTTER = no, then

$$Elocal\_soil_{drift,roof} = AREAroof \cdot Vform \cdot Fform \cdot RHOform \cdot Fdrift_{rinse} \cdot Frinse_i \qquad \mathbf{(273)}$$

$$Elocal\_soil_{drift,\,façade} = AREAfaçade \cdot Vform \cdot Fform \cdot RHOform \cdot Fdrift_{rinse} \cdot Frinse_i \qquad \mathbf{(274)}$$

$$Elocal\_soil_{runoff,roof} = AREA_{roof} \cdot Vform \cdot Fform \cdot RHOform \cdot Frunoff_{rinse} \cdot Frinse_i \qquad \mathbf{(275)}$$

$$Elocal\_soil_{runoff,\,façade} = AREAfaçade \cdot Vform \cdot Fform \cdot RHOform \cdot Frunoff_{rinse} \cdot Frinse_i \qquad \mathbf{(276)}$$

$$Csoil\_adjacent = \frac{Elocal\_soil_{runoff,roof} + Elocal\_soil_{runofft,\,façade}}{Vsoil\_adjacent \cdot RHOsoil} \quad \textbf{(277)}$$

$$Csoil\_distant = \frac{Elocal\_soil_{drift,roof} + Elocal\_soil_{drift,\,façade}}{Vsoil\_distant \cdot RHOsoil} \quad \textbf{(278)}$$

if GUTTER = yes, then

$$Elocal_{7,water} = \frac{AREAroof \cdot Vform \cdot Fform \cdot RHOform \cdot Frunoff_{rinse} \cdot Frinse_i}{Temission_{rinse}} \quad \textbf{(279)}$$

$$Csoil\_adjacent = \frac{Elocal\_soil_{runoff,\,façade}}{Vsoil\_adjacent \cdot RHOsoil} \quad \textbf{(280)}$$

$$Csoil\_distant = \frac{Elocal\_soil_{drift,roof} + Elocal\_soil_{drift,\,façade}}{Vsoil\_distant \cdot RHOsoil} \quad \textbf{(281)}$$

City

$$Elocal_{7,water} = \frac{(AREAroof + AREAfaçade) \cdot Vform \cdot Fform \cdot RHOform \cdot Frinse_i}{Temission_{rinse}} \quad \textbf{(282)}$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_{rinse}$	[d]	1

Input			
Felim	fraction of product eliminated between application and rinse	[-]	D
$Frinse_{spray}$	fraction of product lost during rinse for spraying	[-]	O^c
$Frinse_{roll}$	fraction of product lost during rinse for rolling and brushing	[-]	O^c
$Fdrift_{rinse}$	fraction of product lost during rinse due to spray drift	[-]	D
$Frunoff_{rinse}$	fraction of product lost during rinse due to runoff	[-]	D
$Temission_{rinse}$	number of emission days for rinsing	[d]	D
$Elocal\ \_soil_{drift,roof}$	local emission to soil from spray-drift due to roof rinse	$[kg_c]$	O^c
$Elocal\ \_soil_{drift,façade}$	local emission to soil from spray-drift due to façade rinse	$[kg_c]$	O^c
$Elocal\_soil_{runoff,roof}$	local emission to soil from runoff, due to roof rinse	$[kg_c]$	O^c
$Elocal\_soil_{runoff,\ façade}$	local emission to soil from runoff, due to rinse of façade,	$[kg_c]$	O^c
Output			
$Elocal_{7,water}$	local emission to waste water due to rinse	$[kg_c.d^{-1}]$	O
Csoil-adjacent	local concentration in soil adjacent to building	$[kg_c.kg_{wwt}^{-1}]$	O
Csoil-distant	local concentration in soil distant to building	$[kg_c.kg_{wwt}^{-1}]$	O
Temission	number of emission days	[d]	D

Table III-100 Default settings for roof spraying.

Parameter	**Symbol**	**Unit**	**Value**
Fraction of product eliminated between application and rinse	Felim	[-]	0
Fraction of product lost during rinse due to runoff	$Frunoff_{rinse}$	[-]	0.75
Fraction of product lost during rinse due to spray-drift	$Fdrift_{rinse}$	[-]	0.25
Number of emission days for rinsing	$Temission_{rinse}$	[d]	1

III.3.6.8.4 Masonry preservatives used for in- situ treatment, treated objects

Parameters/variables and default values for release during service life (stage 5).

Countryside

if GUTTER = no, then

$$Csoil\_adjacent_{T1} = \frac{Qleach_{T1} \cdot (AREAfaçade + AREAroof)}{Vsoil\_adjacent \cdot RHOsoil} \quad \textbf{(283)}$$

$$Csoil\_adjacent_{T2} = \frac{Qleach_{T2} \cdot (AREAfaçade + AREAroof)}{Vsoil\_adjacent \cdot RHOsoil} \quad \textbf{(284)}$$

if GUTTER = yes, then

$$Csoil\_adjacent_{T1} = \frac{Qleach_{T1} \cdot AREAfaçade}{Vsoil\_adjacent \cdot RHOsoil} \quad \textbf{(285)}$$

$$Csoil\_adjacent_{T2} = \frac{Qleach_{T2} \cdot AREAfaçade}{Vsoil\_adjacent \cdot RHOsoil} \quad \textbf{(286)}$$

City

$$Elocal_{5,water} = \frac{Nbuilding \cdot Fpenetr \cdot Qleach_{T2} \cdot (AREAfaçade + AREAroof)}{Temission} \quad \textbf{(287)}$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_{ini}$	[d]	30
Temission	$Temission_{chron}$	[d]	365

Input

GUTTER	Building fitted with gutter	[yes/no]	P
AREAfaçade	treated roof area of building	[m^2]	D
AREAroof	treated roof area of building	[m^2]	D
$Qleacht_{T1}$	cumulative quantity of active ingredient leached over the initial assessment period	[$kg_c.m^{-2}$]	S
$Qleacht_{T2}$	cumulative quantity of active ingredient leached over the longer assessment period	[$kg_c.m^{-2}$]	S
$Temission_{ini}$	Duration of the initial assessment period	[d]	D
$Temssion_{chron}$	duration of the longer assessment period	[d]	D
Vsoil-adjacent	volume of soil adjacent to treated object	[m^3]	D
RHOsoil	density of wet soil	[$kg_{wwt}.m^{-3}$]	
Fpenetr	penetration factor	[-]	D
Nbuilding	number of treated buildings in a city	[-]	D
$Elocal\_water_{T1}$	local emission to water from treated building at the countryside during the initial assessment period	[$kg_c.d^{-1}$]	O^c
$Elocal\_water_{T2}$	local emission to water from treated building at the countryside during the longer assessment period	[$kg_c.d^{-1}$]	O^c

Output

$Elocal_{5,water}$	local emission to waste water from treated buildings in a city	[$kg_c.d^{-1}$]	O
$Csoil\text{-}adjacent_{T1}$	local concentration in soil adjacent to façade	[$kg_c.kg_{wwt}^{-1}$]	O
$Csoil\text{-}distant_{T2}$	local concentration in soil distant to façade	[$kg_c.kg_{wwt}^{-1}$]	O
Temission	number of emission days	[d]	O

Table III-101 Default settings for façade spraying.

Parameter	**Symbol**	**Unit**	**Value**
Roof fitted with gutter	GUTTER	[yes/no]	yes
Area of façade treated	AREAfaçade	[m^2]	125
Area of façade treated	AREAroof	[m^2]	145
Cumulative quantity of active ingredient leached over initial assessment period	$Qleach_{T1}$	[$kg.m^{-2}$]	-
Cumulative quantity of active ingredient leached over longer assessment period	$Qleach_{T2}$	[$kg.m^{-2}$]	-
Duration of the initial assessment period	$Temission_{ini}$	[d]	30
Duration of the longer assessment period	$Temission_{chron}$	[d]	>30
Bulk density of wet soil	RHOsoil	[$kg_{wwt}.m^{-3}$]	1700
Volume of soil adjacent to building	Vsoil	[-]	0.5
Penetration factor for product	Fpenetr	[-]	1
Number of treated buildings in a city	Nbuilding	[-]	1

III.3.6.9 Product type 11: Preservatives for liquid-cooling and processing systems

The scenarios and models and calculation formulations used in this version of EUSES 2.1.1 for Preservatives for liquid-cooling and processing systems have been taken from the following document:

- Supplement to the methodology for risk evaluation of biocides Harmonisation of Environmental Emission Scenarios for biocides used as preservatives for liquid cooling systems (product type 11) EC DG ENV / RIVM, 2003

This document can be obtained from the ECB Biocides website

The following modifications are made:

- In order to determine the concentration in surface water depending on the river flow and the blow flow rate, additional equations have been added.
- Furthermore in addition to the original emission scenario the average emission and average concentration have been added to the calculations for the concentration at a certain point in time.
- Also different exposure time frames have been distinguished for the shock dosing scenarios e.g. the acute and chronic situation.

III.3.6.9.1 Biocides in process and cooling-water installations

Industrial use

Parameters/variables and default values for release from once-through systems

Once-through systems can be modeled as plug-flow reactors. The plug leaves the system at the hydraulic residence time. The event lasts for a period which equals the dosing time period. Degradation does only take place during the time the plug is in the system, the hydraulic residence time. Repeated dosing can take place at regular time intervals, several times a day. In that case the average daily concentration in the blowdown should be estimated taking the number of dosings per day into account. For once-through systems release and the concentration are calculated for each dosing event, for the acute situation representing one emission day and the chronic situation representing 300 emission days. The blow down water can either be discharged directly to surface water or the public STP. The latter is usually only the case for small cooling systems. In case of direct discharge the concentration in surface water is directly calculated by applying a dilution factor. The dilution factor, for which no default value is given in the scenario, should be based on the discharge of the total number of cooling systems at the site, Ncool.

General

$$HRT = \frac{Vsyst}{Qbld} \tag{288}$$

$$DILUTION_{cooling} = \frac{FLOW_{river} + N_{cool} \cdot Qbld}{N_{cool} \cdot Qbld} \tag{289}$$

$$\text{When Qbld > Flow river, } DILUTION_{cooling} = 1 \tag{290}$$

Shock dosing event

$$Cproc = \frac{Qform_{event} \cdot Fform}{Qbld \cdot Tdose_{event}} \tag{291}$$

no degradation

$$Cbld = Cproc \tag{292}$$

$$RELEASE_{event} = N_{cool} \cdot Qform_{event} \cdot Fform \tag{293}$$

with degradation

$$Cbld = Cproc \cdot e^{-k\deg \cdot HRT} \tag{294}$$

$$RELEASE_{event} = N \cdot Qform_{event} \cdot Fform \cdot e^{-k\deg \cdot HRT} \tag{295}$$

for both with and without degradation

$$Cwater_{event} = \frac{Cbld}{DILUTION_{cooling}} \tag{296}$$

$$Elocal_{3,air-event} = Fevap \cdot N_{cool} \cdot Cbld \cdot Qbld \cdot Tdose_{event} \tag{297}$$

‘Acute and chronic situation’

$$Ndose = 1/Tint \tag{298}$$

$$Cwater_{acute/chron} = \frac{Cbld \cdot Tdose_{event} \cdot Ndose}{DILUTION_{cooling}} \tag{299}$$

$$Elocal_{3,water} = RELEASE_{event} \cdot Ndose \tag{300}$$

$$Elocal_{3,air} = Fevap \cdot N_{cool} \cdot Cbld \cdot Qbld \cdot Tdose_{event} \cdot Ndose \tag{301}$$

Continuous dosing

$$Cproc = \frac{Qform_{cont} \cdot Fform}{Qbld \cdot HRT} \qquad \textbf{(302)}$$

no degradation

$$Cbld = Cproc \qquad \textbf{(303)}$$

with degradation

$$Cbld = Cproc \cdot e^{-k\deg \cdot HRT} \qquad \textbf{(304)}$$

for both with and without degradation:

$$RELEASE_{cont-T} = N_{cool} \cdot Cbld \cdot Qbld \cdot Temission_{cont} \qquad \textbf{(305)}$$

$$Elocal_{3,water} = N_{cool} \cdot Cbld \cdot Qbld \qquad \textbf{(306)}$$

$$Cwater_{cont} = \frac{Cbld}{DILUTION_{cooling}} \qquad \textbf{(307)}$$

$$Elocal_{3,air-cont} = Fevap \cdot N_{cool} \cdot Cbld \cdot Qbld \qquad \textbf{(308)}$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_{acute}$	[d]	1
Temission	$Temission_{chron}$	[d]	300
Temission	$Temission_{cont}$	[d]	300

Input			
Vsyst	volume of water in cooling system	[m^3]	D
Qbld	blowdown flow rate	[$m^3.d^{-1}$]	D
$Qform_{event}$	amount of product used in shock dose treatment	[kg]	S
$Qform_{cont}$	amount of product applied in continuous treatment during a time period = HRT	[kg]	S
Fform	fraction of substance in the used product	[$kg_c.kg^{-1}$]	S
$Tdose_{event}$	duration of shock dosing event	[d]	D
Ncool	number of cooling systems per site	[-]	D
kdeg	degradation rate constant	[d^{-1}]	S
HRT	hydraulic residence time	[d]	O^c
Cproc	concentration in cooling water of the cooling system	[$kg_c.m^{-3}$]	O
Fevap	fraction of water lost due to evaporation	[-]	D
Cbld	concentration in blow down water	[$kg_c.m^{-3}$]	O
Cproc	concentration in cooling water of the cooling system	[$kg_c.m^{-3}$]	O
Ndose	number of dosings per day	[d^{-1}]	O
Tint	dosing time interval	[d]	S
$FLOW_{river}$	river flow rate	[$m^3.d^{-1}$]	S
$DILUTION_{cooling}$	dilution factor in receiving surface water for the total number of cooling systems (Ncool)	[-]	O/S
$Temission_{cont}$	number of emission days per year	[d]	O
Output			
$RELEASE_{event}$	release from a shock dosing event	[kg_c]	O
$Elocal_{3,air-event}$	local emission to air at shock dose treatment event	[$kg.d^{-1}$]	O
$RELEASE_{cont-T}$	continuous release of substance over time period T	[kg_c]	O
$Elocal_{3,air-cont}$	local emission to air from continuous dosing	[$kg.d^{-1}$]	
$Cwater_{event}$	concentration of chemical in surface water during shock dosing event	[$kg_c.m^{-3}$]	O
$Cwater_{acute/chron}$	concentration of chemical in surface water	[$kg_c.m^{-3}$]	O
$Cwater_{cont}$	average concentration in surface water over *T* days	[$kg_c.m^{-3}$]	O

Table III-102 Default settings of the model for biocides used in once-through process and cooling-water installations.

Parameter	**Symbol**	**Unit**	**Value**
Volume of water in cooling system	Vsyst	[m^3]	6 000
Blow down flow rate	Qbld	[$m^3.d^{-1}$]	576 000
amount of product used in shock dose treatment	$Qform_{event}$	[kg]	-
Fraction of substance in the applied product	Fform	[$kg_c.kg^{-1}$]	-
Duration of shock dose event	$Tdose_{event}$	[d]	0.01042
Number of cooling systems per site	Ncool	[-]	2
Degradation rate constant	kdeg	[d^{-1}]	-
Fraction of water lost due to evaporation	F_{evap}	[-]	0.01
Flow rate of receiving surface water	$FLOW_{river}$	[-]	-
Dilution factor for receiving surface water	$DILUTION_{cooling}$	[-]	-

Parameters/variables and default values for release from open recirculation systems

Open recirculation systems can be modeled as a continuously ideally stirred tank reactor when assuming that the recirculation flow rate (Qcirc) is much larger than the blow down flow rate (Qbld). With a recycle ratio of 50-75 this seems to be justified. For recirculation systems the following output is generated for shock-dosing and continuous dosing: the average concentration and the average emission over a certain period of time can be calculated. Additionally the concentration at the time of sampling can be calculated. For discharge of the blowdown water the same as for once-through systems holds in that that diluation factor should be based on the blowdown flow rate of the total number of cooling systems on-site.

General

$$Qevap\_drift = Qcirc \cdot (Fevap\_drift) \tag{309}$$

$$HRT = \frac{Vsyst}{Qbld + Qevap\_drift} \tag{310}$$

$$Ksyst = \frac{Qbld + Qevap\_drift}{Vsyst} + kdeg \tag{311}$$

Shock dosing

$$Cproc = \frac{Qform_{event} \cdot Fform}{Vsyst} \tag{312}$$

after one shock dose (maximum release period equals Tint, T≤ Tint):

$$Cbld_t = Cproc \cdot e^{-Ksyst \cdot t} \tag{313}$$

$$Cbld_T = Cproc \cdot \frac{(1 - e^{-Ksyst \cdot T})}{Ksyst \cdot T} \tag{314}$$

$$RELEASE_{shock,T} = Qbld \cdot Cproc \cdot \frac{1 - e^{-Ksyst \cdot T}}{Ksyst} \cdot N_{cool} \tag{315}$$

$$RELEASE_{\max} = \frac{Cproc \cdot Qbld}{Ksyst} \cdot N_{cool} \tag{316}$$

no discharge to STP

$$DILUTION_{cooling} = \frac{FLOW_{river} + N_{cool} \cdot Qbld}{N_{cool} \cdot Qbld} \qquad \textbf{(317)}$$

When Qbld > Flow river, $DILUTION_{cooling} = 1$ **(318)**

$$Cwater_{shock,T} = \frac{Cbld_T}{DILUTION_{cooling}} \qquad \textbf{(319)}$$

with discharge to STP

If N_{cool} ·Qbld > 2000 $m^3.d^{-1}$ than: $EFFLUENT_{cooling} = N_{cool} \cdot Qbld$ **(320)**

else, $EFFLUENT_{cooling} = 2000\ m^3 \cdot d^{-1}$

$$Elocal_{3,water} = \frac{RELEASE_{shock,T}}{T} \qquad \textbf{(321)}$$

after n dosings at time intervals Tint, for (t- (i - 1) . Tint) > 0**:**

$$n = T/Tint \qquad \textbf{(322)}$$

$$Cbld_t = \sum_{i=1}^{n} Cproc \cdot e^{-(t-(i-1)\cdot Tint)\cdot Ksyst} \qquad \textbf{(323)}$$

$$Cbld_T = \sum_{i=1}^{n} Cproc \cdot \frac{(1 - e^{-(T-(i-1)\cdot Tint)\cdot Ksyst})}{Ksyst \cdot T} \qquad \textbf{(324)}$$

$$RELEASE_{shock-\mathrm{int},T} = \sum_{i=1}^{n} Qbld \cdot Cproc \cdot \frac{(1 - \mathrm{e}^{-(\mathrm{T}-(\mathrm{i}-1)\cdot \mathrm{Tint})\cdot \mathrm{Ksyst}})}{\mathrm{Ksyst}} \cdot Ncool \qquad \textbf{(325)}$$

no degradation

$$Elocal_{3,air} = Fevap\_drift \cdot Cproc \cdot Qcirc \cdot N_{cool} \qquad \textbf{(326)}$$

$$DOSE_{pest} = \frac{Fdepos \cdot Cproc \cdot Qcirc \cdot N_{cool}}{AREA_{depos}} \tag{327}$$

with degradation

$$Elocal_{3,air} = Fevap\_drift \cdot Cbld_T \cdot Qcirc \cdot N_{cool} \tag{328}$$

$$DOSE_{pest} = \frac{Fdepos \cdot Cbld_T \cdot Qcirc \cdot N_{cool}}{AREA_{depos}} \tag{329}$$

for both with and without degradation

no discharge to STP

$$DILUTION_{cooling} = \frac{FLOW_{river} + N_{cool} \cdot Qbld}{N_{cool} \cdot Qbld} \tag{330}$$

When Qbld > Flow river, $DILUTION_{cooling} = 1$ **(331)**

$$Cwater_{shock-\mathrm{int},T} = \frac{Cbld_T}{DILUTION_{cooling}} \tag{332}$$

with discharge to STP

If $N_{cool} \cdot Qbld > 2000\ m^3.d^{-1}$ than: $EFFLUENT_{cooling} = N_{cool} \cdot Qbld$ **(333)**

else, $EFFLUENT_{cooling} = 2000\ m^3 \cdot d^{-1}$

$$Elocal_{3,water} = \frac{RELEASE_{shock-\mathrm{int},T}}{T} \tag{334}$$

Continuous dosing

$$Cproc = \frac{Qform_{cont} \cdot Fform}{Vsyst} \tag{335}$$

$$Cbld = \frac{Cproc_{init}}{1 + Ksyst \cdot HRT} \tag{336}$$

$$RELEASE_{cont,T} = N_{cool} \cdot Cbld \cdot Qbld \cdot T \tag{337}$$

no degradation

$$Elocal_{3,air} = Fevap - drift \cdot Cproc \cdot Qcirc \cdot N_{cool} \tag{338}$$

$$DOSE_{pest} = \frac{Fdepos \cdot Cproc \cdot Qcirc \cdot N_{cool}}{AREA_{depos}} \tag{339}$$

with degradation

$$Elocal_{3,air} = Fevap\_drift \cdot Cbld \cdot Qcirc \cdot N_{cool} \tag{340}$$

$$DOSE_{pest} = \frac{Fdepos \cdot Cbld \cdot Qcirc \cdot N_{cool}}{AREA_{depos}} \tag{341}$$

no discharge to STP

$$DILUTION_{cooling} = \frac{FLOW_{river} + N_{cool} \cdot Qbld}{N_{cool} \cdot Qbld} \tag{342}$$

When Qbld > Flow river, $DILUTION_{cooling} = 1$ **(343)**

$$Cwater_{cont} = \frac{Cbld}{DILUTION_{cooling}} \tag{344}$$

with discharge to STP

If N_{cool} ·Qbld > 2000 $m^3.d^{-1}$ than: $EFFLUENT_{cooling} = N_{cool} \cdot Qbld$ **(345)**

else, $EFFLUENT_{cooling} = 2000\ m^3 \cdot d^{-1}$

$$Elocal_{3,water} = \frac{RELEASE_{cont,T}}{T} \tag{346}$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
$EFFLUENT_{stp}$	EFFLUENTcooling	[-]	-
DILUTION	$DILUTIONcooling_{small/large}$	[-]	-
Temission	Tshock	[d]	≤ Tint
Temission	Trep-shock	[d]	300
Temission	Tcontinuous	[d]	300

Input

Vsyst	volume of water in cooling system	$[m^3]$	D
Qbld	blowdown flow rate	$[m^3.d^{-1}]$	D
Qcirc	cooling water recirculation flow rate	$[m^3.d^{-1}]$	D
Fevap_drift	fraction of water lost due to evaporation and drift	[-]	D
$Qform_{event}$	amount of product used in shock dose treatment	[kg]	S
$Qform_{cont}$	amount of product used in continuous treatment	$[kg.d^{-1}]$	S
Fform	fraction of substance in the used product	$[kg_c.kg^{-1}]$	S
Cproc	concentration in cooling water of the cooling system	$[kg_c.m^{-3}]$	O
kdeg	degradation rate constant	$[d^{-1}]$	S
n	number of dosings during the emission period	[-]	O
t	time of sampling	[d]	S
Tshock	number of emission days for one shock dosing	[d]	S
Trep-shock	number of emission days for repeated shock dosing	[d]	S
Tcontinuous	number of emission days for continuous dosing	[d]	S
Ncool	number of cooling systems per site	[-]	D
Tint	time period between two emission events	[d]	D
HRT	hydraulic residence time	[d]	O
Qevap_drift	amount of cooling water lost due to evaporation and drift	$[m^3.d^{-1}]$	
Ksyst	overall rate constant for removal from the cooling system	$[d^{-1}]$	O
$Cbld_t$	concentration in blow down water at time t	$[kg_c.m^{-3}]$	O
$Cbld_T$	concentration in blow down water after time period T	$[kg_c.m^{-3}]$	O
Cbld	concentration in blow down water	$[kg_c.m^{-3}]$	O
$AREA_{depos}$	surface area for soil where deposition occurs	$[m^2]$	D
Fdepos	fraction of water lost due to drift and reaching soil	[-]	D
$EFFLUENT_{cooling}$	Eflluent discharge rate for the total number of cooling systems at the site (Ncool)	[-]	O
$DILUTION_{cooling}$	dilution factor in receiving surface water for the total number of cooling systems at the site (Ncool)	[-]	S/O
$RELEASE_{shock,T}$	total release over time period T from one shock dosing event	$[kg_c]$	O
$RELEASE_{max}$	maximum release from shock dosing after infinite time	$[kg_c]$	O
$RELEASE_{shock\text{-}int,T}$	total release over time period T from multiple shock dosing events	$[kg_c]$	O
$RELEASE_{cont,T}$	total amount of substance released at continuous dosing after time period T	$[kg_c.^{d-1}]$	O

Output

$Elocal_{3,air}$	local emission to air	$[kg.d^{-1}]$	O
$Elocal_{3,water}$	local (average) emission to (waste) water	$[kg.d^{-1}]$	O
DOSEpest	Dose of active ingredient to soil	$[kg_c.m^{-2}.d^{-1}]$	O
$Cwater_{cont}$	average concentration in water over time periode T	$[kgc.m^{-3}]$	O
$Cwater_{shock,T}$	average concentration of chemical in surface water after on shock dose event	$[kg_c.m^{-3}]$	O
$Cwater_{shock\text{-}int,T}$	average concentration in surface water over *T* days	$[kg_c.m^{-3}]$	O

Table III-103 Default settings of the model for biocides used in small and large open recirculation process and cooling-water installations.

Parameter	**Symbol**	**Unit**	**Value** **large**	 **small**
Volume of water in cooling system	Vsyst	[m^3]	3 000	300
Blow down flow rate	Qbld	[$m^3.d^{-1}$]	3 000	48
Recirculation flow rate for cooling water	Qcirc	[$m^3.d^{-1}$]	216 000	2 400
Fraction of water released due to evaporation and drift	Fevap_drift	[-]	0.01	0.01
amount of product used in shock dose treatment	$Qform_{event}$	[kg]	-	
Number of cooling systems per site	Ncool	[-]	2	
Time period between two emission event	Tint	[d]	1	
Fraction of water lost due to drift and reaching soil	F_{depos}	[-]	0.00025	
Soil surface area where deposition occurs	$AREA_{depos}$	[m^2]	100	
Dilution factor for receiving surface water	$DILUTION_{cooling}$	[-]		

Parameters/variables and default values for release from closed systems

Single dosing

$$Cproc = \frac{Qform_{event} \cdot Fform}{Vsyst} \tag{347}$$

$$HRT = \frac{Vsyst}{Qbld} \tag{348}$$

$$Ksyst = \frac{1}{HRT} + k\deg \tag{349}$$

after one shock dose (maximum release period equals Tint, T≤ Tint):

$$Cbld_t = Cproc \cdot e^{-Ksyst \cdot t} \tag{350}$$

$$Cbld_T = Cproc \cdot \frac{1 - e^{-Ksyst \cdot T}}{Ksyst \cdot T} \tag{351}$$

$$RELEASE_{shock,T} = Cproc \cdot Qbld \cdot \frac{1 - e^{-Ksyst \cdot T}}{Ksyst} \cdot Ncool \tag{352}$$

$$RELEASE_{\max} = \frac{Cproc \cdot Qbld}{Ksyst} \cdot Ncool \tag{353}$$

$$DILUTION_{cooling} = \frac{FLOW_{river} + N_{cool} \cdot Qbld}{N_{cool} \cdot Qbld} \tag{354}$$

When Qbld > Flow river, $DILUTION_{cooling} = 1$ **(355)**

$$Cwater_{shock,T} = \frac{Cbld_T}{DILUTION_{cooling}} \tag{356}$$

no degradation

$$RELEASE_{dosing} = Fdosing \cdot Vsyst \cdot Cproc \tag{357}$$

$$RELEASE_{design} = Fdesign \cdot Vsyst \cdot Cproc \tag{358}$$

$$RELEASE_{drainage} = Fdrainage \cdot Vsyst \cdot Cproc \tag{359}$$

after n dosings at time intervals Tint, **for (T- (i - 1) . Tint) > 0**:

$$n = T/Tint \tag{360}$$

$$Cbld_t = \sum_{i=1}^{n} Cproc \cdot e^{-(t-(i-1)Tint) \cdot Ksyst} \tag{361}$$

$$Cbld_T = \sum_{i=1}^{n} Cproc \cdot \frac{1 - e^{-(T-(i-1)Tint) \cdot Ksyst}}{Ksyst \cdot T} \tag{362}$$

$$RELEASE_{shock-\mathrm{int},T} = \sum_{i=1}^{n} Qbld \cdot Cproc \cdot \frac{(1 - e^{-(T-(i-1) \cdot Tint) \cdot Ksyst})}{Ksyst} \cdot Ncool \tag{363}$$

For both with and without degradation:

direct discharge to surface water

$$DILUTION_{cooling} = \frac{FLOW_{river} + N_{cool} \cdot Qbld}{N_{cool} \cdot Qbld} \tag{364}$$

$$\text{When Qbld > Flow river, } DILUTION_{cooling} = 1 \tag{365}$$

$$Cwater_{shock-\text{int},T} = \frac{Cbld_T}{DILUTION_{cooling}} \tag{366}$$

discharge to STP

$$\text{If } N_{cool} \cdot Qbld > 2000\ m^3.d^{-1} \text{ than: } EFFLUENT_{cooling} = N_{cool} \cdot Qbld \tag{367}$$

$$\text{else, } EFFLUENT_{cooling} = 2000\ m^3 \cdot d^{-1}$$

$$Elocal_{3,water} = \frac{RELEASE_{cont,T}}{T} \tag{368}$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
$EFFLUENT_{stp}$	EFFLUENTcooling	[-]	-
DILUTION	$DILUTIONcooling_{small/large}$	[-]	-
Temission	Tshock	[d]	≤ Tint
Temission	Trep-shock	[d]	300

Input

Vsyst	volume of water in cooling system	[m^3]	D
Qbld	blowdown flow rate	[$m^3.d^{-1}$]	D
$Qform_{event}$	amount of product used in shock dose treatment	[kg]	S
Fform	fraction of substance in the used product	[$kg_c.kg^{-1}$]	S
Cproc	concentration in cooling water of the cooling system	[$kg_c.m^{-3}$]	O
kdeg	degradation rate constant	[d^{-1}]	S
n	number of dosings during the emission period	[-]	O
t	time of sampling	[d]	S
Tshock	number of emission days for a single shock dosing	[d]	S
Trep-shock	number of emission days for repeated shock dosing	[d]	S
Ncool	number of cooling systems per site	[-]	D
Fdosing	fraction of the substance lost during dosing event	[-]	D
Fdesign	fraction of the substance lost due to design	[d^{-1}]	D
Fdrainage	fraction of the substance lost at complete drainage	[-]	D
Tint	time period between two dosing events	[d]	D
HRT	hydraulic residence time	[d]	O
Ksyst	overall rate constant for removal from the cooling system	[d^{-1}]	O
$Cbld_t$	concentration in blow down water at time t	[$kg_c.m^{-3}$]	O
$Cbld_T$	average concentration in blow down water over time period T	[$kg_c.m^{-3}$]	O
$EFFLUENT_{cooling}$	Eflluent discharge rate for the total number of cooling systems at the site (Ncool)	[-]	O
$DILUTION_{cooling}$	dilution factor in receiving surface water for the total number of cooling systems at the site (Ncool)	[-]	O/S
$RELEASE_{shock,T}$	total release over time period T from one shock dosing event	[kg_c]	O
$RELEASE_{max}$	maximum release from shock dosing after infinite time	[kg_c]	O

$RELEASE_{shock\text{-}int,T}$	total release over time period T from multiple shock dosing events	$[kg_c]$	O
Output			
$RELEASE_{dosing}$	release from one dosing event	$[kg_c]$	O
$RELEASE_{design}$	average design losses	$[kg_c.d^{-1}]$	O
$RELEASE_{drainage}$	release from drainage, per event	$[kg_c]$	O
$Cwater_{shock,T}$	average concentration of chemical in surface water after one dosing event	$[kg_c.m^{-3}]$	O
$Cwater_{shock\text{-}int,T}$	average concentration in surface water over *T* days	$[kg_c.m^{-3}]$	O
$Elocal_{3,water}$	local emission to waste water	$[kg.d^{-1}]$	O

Table III-104 Default settings of the model for biocides used in small and large open recirculation process and cooling-water installations.

Parameter	**Symbol**	**Unit**	**Value**
Volume of water in cooling system	Vsyst	$[m^3]$	30
Blow down flow rate	Qbld	$[m^3.d^{-1}]$	0.0096
amount of product used in shock dose treatment	$Qform_{event}$	[kg]	-
Fraction of substance in the applied product	Fform	$[kg_c.kg^{-1}]$	-
Number of cooling systems per site	Ncool	[-]	1
Fraction lost during dosing	Fdosing	[-]	0.005
Fraction lost due to design	Fdesign	$[d^{-1}]$	0.00033
Fraction lost at complete drainage	Fdrainage	[-]	1
Degradation rate constant	Kdeg	$[d^{-1}]$	-
Time period between two emission event	Tint	[d]	-
Fraction of water lost due to drift and reaching soil	F_{depos}	[-]	0.00025
Soil surface area where deposition occurs	$AREA_{depos}$	$[m^2]$	100
Dilution factor for receiving surface water	$DILUTION_{cooling}$	[-]	-

III.3.6.10 Product type 12: Slimicides

The scenarios and models and calculation formulations used in this version of EUSES 2.1.1 for slimicides have been taken from the following document:

- Supplement to the methodology for risk evaluation of biocides Harmonisation of Environmental Emission Scenarios for slimicides (product type 12) (EC DG ENV / RIVM, 2003

This document can be obtained from the ECB Biocides website

The following modifications are made:

- The exposure duration, test duration of toxicity is set equal to the number of emission days.
- Furthermore in addition to the original emission scenario the average emission and average concentration have been added to the calculations for the concentration at a certain point in time.
- Also different exposure time frames have been distinguished for the shock dosing scenarios e.g. the acute and chronic situation.

III.3.6.10.1 Slimicides used in paper mills

Release of slimicide in paper mills not taking degradation into account

$$Qsubst = Qform_{uins} \cdot Cform \ / \ RHOform \tag{369}$$

A) based on amount of active ingredient per unit of mass of dry paper

$$Cinf = Qsubst/Vww \cdot (1 - Floss) \tag{370}$$

B) based on amount of active ingredient per unit of volume of process water

$$Cinf = Qsubst \cdot Fww1 \cdot \left(1 - Fww2\right) \cdot (1 - Floss) \tag{371}$$

C) based on prescribed concentration in process water

$$Cinf = Cproc \cdot Fww1 \cdot \left(1 - Fww2\right) \cdot (1 - Floss) \tag{372}$$

$$Elocal_{3,water} = EFFLUENT_{stp} \cdot Cinf \tag{373}$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_3$	[d]	300
Nlocal	$Nlocal_3$	[eq]	25,000
DILUTION	$DILUTION_3$	[-]	-

Input			
Qform_uins	amount of biocide prescribed in user's instructions for one tonne of dry paper or per m^3 process water	[kg]	S
Cform	content of active ingredient in biocidal product	$[kg_c.m^{-3}]$	S
RHOform	specific density of biocide formulation	$[kg.m^{-3}]$	S
Vww	amount of waste water per kilogram of dry paper	$[m^3.kg^{-1}]$	D
APPL	treatment of both long and short circulation with slimicide	[yes/no]	P
Fww1	fraction of the total waste water flow coming from the short circulation of the wire part	[-]	O
CONN	connection to pulp mill	[yes/no]	P
Fww2	fraction dilution of waste water with waste water from pulping	[-]	O
Cproc	concentration in process water prescribed in the user's instructions	$[kg.m^{-3}]$	S
Qsubst	amount of active ingredient per kilogram of dry paper	$[kg_c.kg^{-1}]$	O
Floss	total fraction of biocide lost in the dry end of the paper making machine	[-]	D
Cinf	theoretical concentration of active ingredient in effluent from paper mill (influent waste water treatment plant)	$[kg.m^{-3}]$	O
$EFFLUENTlocal_{stp}$	effluent discharge of STP for paper plant	$[m^3.d^{-1}]$	D
$Temission_3$	number of emission days	[d]	D
$Nlocal_3$	capacity of local STP of paper plant	[eq]	D
$DILUTION_3$	dilution factor for receiving surface water	[-]	S
Output			
Nlocal	capacity of the local STP	[eq]	O
Temission	number of emission days	[d]	O
DILUTION	dilution factor	[-]	O
$Elocal_{3,water}$	local emission to waste water during episode	$[kg.d^{-1}]$	O

Table III-105 Default settings for calculating the daily release to the STP excluding biodegradation

Parameter	**Symbol**	**Unit**	**Value**
Specific density of biocide formulation	RHOform	$[kg.m^{-3}]$	1,000
Amount of waste water per kilogram of dry paper	Vww	$[m^3]$	0.015
Treatment of both long and short circulation with slimicide	APPL	[yes/no]	yes
Fraction of the total waste water flow coming from the short circulation of the wire part APPL = yes APPL = no	Fww1	[-]	 1 0.6
Connection of pulp mill	CONN	[yes/no]	no
Fraction dilution of waste water with waste water from pulping CONN = yes CONN = no	Fww2	[-]	 0.5 0.0
Fraction of the biocide lost in the dry end of the paper making machine	Floss	[-]	0.1
Effluent discharge of WWTP for paper plant	$EFLLUENTlocal_{stp}$	$[m^3.d^{-1}]$	5,000

Release of slimicides in paper mills taking degradation into account

Calculating rate constants for hydrolysis

$$khydr_{acid} = ln\,2\ /\ DT50hydr_{acid} \quad (374)$$

$$khydr_{water} = ln\,2\ /\ DT50hydr_{water} \quad (375)$$

$$khydr_{alkal} = ln\,2\ /\ DT50hydr_{alkal} \quad (376)$$

Degradation test

$$ktot_{water} = ln\,2\ /\ DT50_{water} \quad (377)$$

Input			
$DT50hydr_{acid}$	half-life time for hydrolysis in acid circumstances	[d]	S
$DT50hydr_{water}$	half-life time for hydrolysis in neutral circumstances	[d]	S
$DT50hydr_{alkal}$	half-life time for hydrolysis in alkaline circumstances	[d]	S
$DT50_{water}$	half-life time for degradation (hydrolysis and biodegradation) in water	[d]	S
Output			
$ktot_{water}$	rate constant for (total) degradation in water	[d^{-1}]	O
$khydr_{water}$	rate constant for degradation due to hydrolysis at neutral (pH≈7) conditions	[d^{-1}]	O
$khydr_{acid}$	rate constant for degradation due to hydrolysis at acid (pH≈5) conditions	[d^{-1}]	O
$khydr_{alkal}$	rate constant for degradation due to hydrolysis at alkaline (pH≈8) conditions	[d^{-1}]	O

Calculating emission to waste water and PECs

concentrations after primary settling

continuous dosing

$$Cacid = Cinf \cdot \frac{1}{1 + khydr_{acid} \cdot Tpr} \cdot e^{-ktot_{water} \cdot Tps} \cdot (1 - Fads_{PS}) \quad (378)$$

$$Cneutr = Cinf \cdot \frac{1}{1 + khydr_{water} \cdot Tpr} e^{-ktot_{water} \cdot Tps} \cdot (1 - Fads_{PS}) \quad (379)$$

$$Calkal = Cinf \cdot \frac{1}{1 + khydr_{alkal} \cdot Tpr} e^{-ktot_{water} \cdot Tps} \cdot (1 - Fads_{PS}) \quad (380)$$

shock dosing, after n dosings at time interval Tint, **for (T- (i - 1) . Tint) > 0**

$$n = Temission_3 / Tint \quad (381)$$

$$Cacid = Cinf \cdot \sum_{i=1}^{n} \frac{1 - e^{-(T - (i-1) \cdot Tint) \cdot khydr_{acid}}}{khydr_{acid} \cdot T} \cdot e^{-ktot_{water} \cdot Tps} \cdot (1 - Fads_{PS}) \quad (382)$$

$$Cneutr = Cinf \cdot \sum_{i=1}^{n} \frac{1 - e^{-(T - (i-1) \cdot Tint) \cdot khydr_{water}}}{khydr_{water} \cdot T} \cdot e^{-ktot_{water} \cdot Tps} \cdot (1 - Fads_{PS}) \quad (383)$$

$$Calkal = Cinf \cdot \sum_{i=1}^{n} \frac{1 - e^{-(T - (i-1) \cdot Tint) \cdot khydr_{alkal}\ )}}{khydr_{alkal} \cdot T} \cdot e^{-ktot_{water} \cdot Tps} \cdot (1 - Fads_{PS}\ ) \tag{384}$$

general calculation for both continuous and shock dosing

concentrations after chemical/mechanical treatment (worst case)

$$Cacid_{CM} = Cacid \cdot e^{-ktot_{water} \cdot Tcm} \cdot (1 - Fads_{CM}\ ) \tag{385}$$

$$Cneutr_{CM} = Cneutr \cdot e^{-ktot_{water} \cdot Tcm} \cdot (1 - Fads_{CM}\ ) \tag{386}$$

$$Calkal_{CM} = Calkal \cdot e^{-ktot_{water}\ ) \cdot Tcm} \cdot (1 - Fads_{CM}\ ) \tag{387}$$

Clocal in receiving surface water after chemical/mechanical treatment

$$Clocal_{CM\_water\_acid} = Cacid_{CM} \div DILUTION \tag{388}$$

$$Clocal_{CM\_water\_neutr} = Cneutr_{CM} \div DILUTION \tag{389}$$

$$Clocal_{CM\_water\_alkal} = Calkal_{CM} \div DILUTION \tag{390}$$

Emission to waste water after primary settling (typical case)

$$Elocal_{3,water,acid} = EFFLUENT_{stp} \cdot Cacid \tag{391}$$

$$Elocal_{3,water,neutr} = EFFLUENT_{stp} \cdot Cneutr \tag{392}$$

$$Elocal_{3,water,alkal} = EFFLUENT_{stp} \cdot Calkal \tag{393}$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_3$	[d]	300
Temission	T	[d]	-
Nlocal	$Nlocal_3$	[eq]	25,000
DILUTION	$DILUTION_3$	[-]	-

Input

Cinf	theoretical concentration of active ingredient	[kg.m^{-3}]	O
Tpr	retention time for paper making process	[d]	D
Tps	retention time for primary settling	[d]	D
Tcm	retention time for chemical/mechanical treatment	[d]	D
$Fads_{PS}$	fraction of the biocide adsorbed to particles during primary settling	[-]	D
$Fads_{CM}$	fraction of the biocide adsorbed to particles during chemical/mechanical treatment	[-]	D
Cacid	concentration after primary settling for acid process conditions	[kg.m^{-3}]	O
Cneutr	concentration after primary settling for neutral process conditions	[kg.m^{-3}]	O
Calkal	concentration after primary settling for alkaline process conditions	[kg.m^{-3}]	O
$Cacid_{CM}$	concentration after chemical/mechanical treatment for acid process conditions	[kg.m^{-3}]	O
$Cneutr_{CM}$	concentration after chemical/mechanical treatment for neutral process conditions	[kg.m^{-3}]	O

$Calkal_{CM}$	concentration after chemical/mechanical treatment for alkaline process conditions	[kg.m^{-3}]	O
$Temission_3$	Number of emission days	[d]	S
Tint	time period between two dosing events	[d]	S
n	number of dosings during the emission period	[-]	O
$EFFLUENTlocal_{stp}$	effluent discharge of STP for paper plant	[m^3.d^{-1}]	D
$Temission_3$	number of emission days	[d]	D
$Nlocal_3$	capacity of local STP of paper plant	[eq]	D
$DILUTION_3$	dilution factor for receiving surface water	[-]	S
Output			
$Clocal_{CM\_water\_acid}$	predicted Environmental Concentration in receiving surface water after chemical/mechanical treatment for acid process conditions at paper making	[kg.m^{-3}]	O
$Clocal_{CM\_water\_alkal}$	predicted Environmental Concentration in receiving surface water after chemical/mechanical treatment for alkaline process conditions at paper making	[kg.m^{-3}]	O
$Clocal_{CM\_water\_neutr}$	predicted Environmental Concentration in receiving surface water after chemical/mechanical treatment for neutral process conditions at paper making	[kg.m^{-3}]	O
Nlocal	capacity of the local STP	[eq]	O
Temission	number of emission days	[d]	O
DILUTION	dilution factor	[-]	O
$Elocal_{3,water,acid}$	local emission to waste water for acid process conditions after primary settling only	[kg.d^{-1}]	O
$Elocal_{3,water,alkal}$	local emission to waste water for alkaline process conditions after primary settling only	[kg.d^{-1}]	O
$EClocal_{3,water,neutr}$	local emission to waste water for neutral process conditions after primary settling only	[kg.d^{-1}]	O

Table III-106 Default settings for calculating the effluent concentrations for on-site treatment and influent concentrations for the STP.

Parameter	**Symbol**	**Unit**	**Value**
Retention time for the paper making process	Tpr	[d]	0.167
Retention time for primary settling	Tps	[d]	0.167
Retention time for chemical/mechanical treatment	Tcm	[d]	0.167
Fraction of the slimicide adsorbed to particles during primary settling	$Fads_{PS}$	[-]	0
Fraction of the biocide adsorbed to particles during chemical/mechanical treatment	$Fads_{CM}$	[-]	0

III.3.6.10.2 Slimicides used in oil extraction processes

Model for release from oil extraction platforms

A) based on the fraction of active ingredient in drilling mud

$$RELEASEwater = Fsubst\_mud \cdot Vmud \cdot RHOmud \tag{394}$$

B) based on amount of active ingredient per unit of volume of drilling mud

$$RELEASEwater = Qsubst\_mud \cdot Vmud \cdot Fconv \tag{395}$$

A/B)

$$Vwater_{platform} = 1/DENSEplatform \cdot DEPTHlocal\_wway \tag{396}$$

$$Vrepl_{water} = Vwater_{platform} \cdot Frepl_{water} \tag{397}$$

Continuous discharge

$$PEClocal_{water,cont} = \frac{RELEASEwater}{Tdrill \cdot Vrepl_{water}} \tag{398}$$

$$Fdeg_{sed} = 1 - e^{-kdeg_{sed} \cdot Tint} \tag{399}$$

$$PEClocal_{sediment} = PEClocal_{water,cont} \cdot Kp_{sed} \cdot (1 - Fdeg_{sed}) \tag{400}$$

Batchwise discharge

$$PEClocal_{water,batch} = \frac{RELEASEwater}{Vmud \cdot DILUTION_{batch}} \tag{401}$$

Parameters/variables and default values for release from oil extraction platforms

Input

-	Type of discharge	[-]	P
-	size of the section	[-]	P
Vmud	volume of mud discharged from a specific section	[m^3]	D
Fsubst_mud	fraction of substance in the mud	[kg$_c$.kg^{-1}]	S
RHOmud	density of the discharged drilling mud	[kg.m^{-3}]	D
Qsubst_mud	amount of substance in drilling mud	[pound.barrel^{-1}]	S
Fconv	conversion factor from pounds per barrel to kg.m^{-3}	[$^{1)}$]	D^c
DENSEplatform	number of platforms per square kilometer	[km^{-2}]	
	DDEPTHlocal_water	average depth of water	
around platform	[m]	D	
Frepl$_{water}$	fraction of sea water refreshed in the receiving volume around the platform per day	[d^{-1}]	D
Tdrill	drilling time for a section	[d]	D
DILUTION$_{batch}$	dilution factor for batch wise discharges	[-]	D
Kp$_{sed}$	sediment water partition coefficient	[m^{-3}.kg^{-1}]	O^c
Vwater$_{platform}$	volume of water around a platform	[m^{-3}]	O
Vrepl$_{water}$	volume of water passing the platform	[m^3.d^{-1}]	O
RELEASEwater	local release of substance to sea water per drilling period	[kg$_c$]	O
CONVsed	conversion factor for sediment concentrations: wwt to dwt	[kg$_{wwt}$.kg$_{dwt}$$^{-1}$]	O]
kdeg$_{sed}$	first order degradation rate in sediment	[d^{-1}]	S
Tint	long term interval for sediment concentration	[d]	D
Fdeg$_{sed}$	fraction of substance in sediment degraded after one year	[-]	O
Kp$_{sed}$	sediment water partition coefficient	[m^3.kg^{-1}]	O

Output

$PEC_{water,cont}$	predicted environmental concentration in receiving sea water for continuous discharges	$[kg_c.m^{-3}]$	O
$PEC_{water,batch}$	predicted environmental concentration in receiving sea water for batch wise discharges	$[kg_c.m^{-3}]$	O
$PEC_{sediment}$	predicted environmental concentration in marine sediment	$[kg_c.kg_{dwt}^{-1}]$	O

[1)] unit of conversion factor is in $[kg.pnd^{-1}.barrel.m^{-3}]$

Table III-107 Default settings for calculating the daily release to the STP excluding biodegradation

Parameter	Symbol	Unit	Value
volume of mud discharged from a specific section	Vmud	$[m^3]$	
continuous discharge			
section 17.5”			600
section 12.25”			450
section 8.5”			250
batch wise discharge			
section 12.25”			375
section 8.5”			280
Fraction of the substance in drilling mud	Fsubst_mud	$[kg_c.kg^{-1}]$	-
Amount of the substance in drilling mud	Qsubst_mud	$[kg.m^{-3}]$	-
Specific density of drilling mud	RHOmud	$[kg.m^{-3}]$	
section 17.5”			1,400
section 12.25”			1,600
section 8.5”			1,600
Conversion factor for pounds per barrel to kg.m-3	Fconv	$[kg.pound^{-1}.barrel.m^{-3}]$	2.853
Number of platforms per square kilometer	DENSEplatform	$[m^{-2}]$	1.10^{-7}
Average depth of water around platform	DEPTHwater	[m]	150
Fraction of the sea water around platform refreshed per day	$Frepl_{water}$	$[d^{-1}]$	0.24
Time needed to drill a section	Tdrill	[d]	16
Dilution factor for batch wise discharges	$DILUTION_{batch}$	[-]	13,000
First order degradation rate for sediment	$Fdeg_{sed}$	$[d^{-1}]$	-
Long term interval for sediment concentration	Tint	[d]	365

III.3.6.11 Product type 13: Metal working-fluid preservatives

The scenarios and models formulations used in this version of EUSES 2.1.1 for metal working fluid preservatives have been taken from the following document:

- Supplement to the methodology for risk evaluation of biocides Harmonisation of Environmental Emission Scenarios for biocides used as metalworking fluid preservatives (Product type 13) (EC DG ENV / RIVM, 2003), which was already implement in EUSES 2.0 (EC, 2004).

This document can be obtained from the ECB Biocides website

A) water-based cooling lubricants:

A.1) cooling lubricants based on emulsions

$$Elocal_{6,water} = \frac{Fproc}{Fproc+1} \cdot \frac{Cconc \cdot Vproc}{Fproc \cdot K_{ow}+1} \cdot Frel \cdot (1-Felim) \cdot (1-Fdeg) \qquad \textbf{(402)}$$

$$Cconc = Fconc \cdot RHOconc \qquad \textbf{(403)}$$

Input			
Cconc	concentration of the substance in the concentrate	$[kg_c.m^{-3}]$	S/O
Fconc	fraction of substance in concentrate	[-]	S/P
RHOconc	density of the concentrate	$[kg.m^{-3}]$	D
Vproc	volume of processed liquid treated in recovery unit	$[m^3.d^{-1}]$	D
Fproc	fraction of concentrate in processed liquid	[-]	S/P
K_{ow}	octanol-water partition coefficient	[-]	S
Felim	fraction of the substance eliminated during treatment	[-]	D
Fdeg	fraction of the substance degraded during industrial use	[-]	D
Frel	factor of relevance	[-]	D
Output			
$Elocal_{6,water}$	local emission to wastewater	$[kg_c.d^{-1}]$	O

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_3$	[d]	300

Table III-108 Defaults for emission calculations.

Parameter	**Symbol**	**Unit**	**Value**
Fraction of substance in concentrate	Fconc	[-]	[1]
Density of concentrate	RHOconc	[kg.m^{-3}]	1000
Volume of processed liquid treated in recovery plant	Vproc	[m^3.d^{-1}]	200
Fraction of concentrate in processed liquid	Fproc	[-]	[2]
Octanol-water partition coefficient	K_{ow}	[-]	[3]
Fraction of the substance eliminated during treatment	Felim	[-]	0
Fraction of the substance degraded during industrial use	Fdeg	[-]	0
Factor of relevance	Frel	[-]	1

[1] see pick-list

Table III-110.

[2] see pick-list ***Table III-111***

[3] substance specific property

A.2) water-soluble lubricants:

$$Elocal_{6,water} = Cconc \cdot Vproc \cdot Fproc \cdot Frel \cdot (1 - Felim) \cdot (1 - Fdeg) \qquad \textbf{(404)}$$

$$Cconc = Fconc \cdot RHOconc \qquad \textbf{(405)}$$

Input

Cconc	concentration of substance in concentrate	[kg$_c$.m^{-3}]	S/O
Fconc	fraction of substance in concentrate	[-]	S/P
RHOprod	density of concentrate	[kg.m^{-3}]	D
Vproc	volume of processed liquid treated in recovery unit	[m^3.d^{-1}]	D
Fproc	fraction of concentrate in processed liquid	[-]	S/P
Felim	fraction of the substance eliminated during treatment	[-]	D
Fdeg	fraction of the substance degraded during industrial use	[-]	D
Frel	factor of relevance	[-]	D

Output

$Elocal_{6,water}$	local emission to wastewater	[kg$_c$.d^{-1}]	O

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_3$	[d]	300

Table III-109 Defaults for emission calculations.

Parameter	**Symbol**	**Unit**	**Value**
Concentration of substance in concentrate	Cconc	[$kg_c.m^{-3}$]	
Fraction of substance in concentrate	Fconc	[-]	1)
Density of concentrate	RHOconc	[$kg.m^{-3}$]	1000
Volume of processed liquid treated in recovery plant	Vproc	[$m^3.d^{-1}$]	40
Fraction of concentrate in processed liquid	Fproc	[-]	2)
Fraction of the substance eliminated during treatment	Felim	[-]	0.8
Fraction of the substance degrade during industrial use	Fdeg	[-]	0
Factor of relevance	Frel	[-]	1

1) see pick-list ***Table III-110***

2) see pick-list ***Table III-111***

Table III-110 Pick-list for composition of cooling lubricants. Fraction of substance in concentrate, Fconc (-). The highest value is chosen to represent the worst case situation.

Substance group	**traditional SEM**^{1}	**synthetic SEM**^{1}	**SES**^{2}
boric acids (biocide)	-	0-0.03	-
Bactericide	0.04	0-0.05	0.03-0.04
Fungicide	0-0.01	0-0.01	0-0.01

1) SEM emulsifiable cooling lubricant

2) SES water soluble cooling lubricant

Table III-111 Pick-list for fraction of cooling lubricant concentrate in processed liquid, Fproc (-) by type of process. In case of a range the highest content is used as the worst case value.

Process	**Content [-]**
Broaching	0.10-0.20
thread cutting	0.05-0.10
deep hole drilling	0.10-0.20
parting-off	0.05-0.10
milling, cylindrical milling	0.05-0.10
turning, drilling, automation work	0.03-0.10
Sawing	0.05-0.20
tool grinding	0.03-0.06
cylindrical grinding	0.02-0.05
centreless grinding	0.03-0.06
surface grinding	0.02-0.05

B) Pure oils cooling lubricants

The scenario assumes no losses to the environment from industrial use as well as waste treatment. In the use stage washing water is processed and the unusable part is disposed of as chemical waste. Used product may be recovered by dripping off, centrifuging and blowing off the chips. Recovered product may be disposed of or reused depending on the degree of contamination of the oil. Highly contaminated oil is disposed of in special refuse incinerators.

III.3.6.12 Product type 14: Rodenticides

The scenarios and equations used in this version of EUSES 2.1.1 for rodenticides have been taken from the following document:

- Supplement to the methodology for risk evaluation of biocides Harmonisation of Environmental Emission Scenarios for biocides used as rodenticides (Product type 14) (EC DG ENV / RIVM, 2003)

This document can be obtained from the ECB Biocides website

The following addition is made:
In the ESD no method is given to determine the risk characterisation ratio (RCR) for secondairy poisoning. This formula has been added. For primairy poisoning no RCR is determined.

III.3.6.12.1 Products used for control in sewer systems

Parameters/variables and default values for wax blocks used in a sewer system.

$$Qprod = Nblock \cdot Qblock \qquad \textbf{(406)}$$

$$F_{3,water} = 0.3 + (0.6 - Fmetab) \qquad \textbf{(407)}$$

$$Elocal_{3,water} = \frac{Qprod \cdot Fsubst \cdot F_{3,water}}{Temission_{contr}} \qquad \textbf{(408)}$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_{contr}$	[d]	7

Input			
Qblock	weight of one wax block	[kg]	D/S
Nblock	number of wax blocks applied	[-]	D/S
Qprod	amount of product used in control operation of one week	[kg]	O/S
Fsubst	fraction of active substance in product	$[kg_c.kg^{-1}]$	S
$Temission_{contr}$	number of emission days during the control operation	[d]	D
Fmetab	fraction of active ingredient metabolised	[-]	D/S
$F_{3,water}$	fraction of active substance released	[d]	O
Output			
$Elocal_{3,water}$	local emission to waste water during episode	$[kg_c.d^{-1}]$	O
Temission	number of emission days	[d]	O

Table III-112 Default settings of the model for rodenticides used in sewer systems.

Parameter	**Symbol**	**Unit**	**Value**
Weight of one wax block	Qblock	[kg]	0.3
Number of wax blocks applied	Nblock	[-]	100
Fraction of active substance in product	Fsubst	$[kg_c.kg^{-1}]$	-
Number of emission days for control operation	$Temission_{contr}$	[d]	7
Fraction of active substance metabolised	Fmetab	[-]	0

III.3.6.12.2 Products used for control around buildings

Parameters/variables and default values for release through use of bait boxes.

Direct release

$$Clocal\_soil_{direct} = \frac{Qprod \cdot Fsubst \cdot Nsites \cdot Nrefill \cdot Fdirect_{soil}}{AREA_{expo,direct} \cdot DEPTHsoil \cdot RHOsoil \cdot Nsites} \qquad \textbf{(409)}$$

Indirect release (via excretion)

$$Fexcr_{soil} = 0.3 + (0.6 - Fmetab) \qquad \textbf{(410)}$$

$$Clocal\_soil_{indirect} = \frac{Qprod \cdot Fsubst \cdot Nsites \cdot Nrefill \cdot Fexcrete_{soil} \cdot (1 - Fdirect_{soil})}{AREA_{expo,indirect} \cdot DEPTHsoil \cdot RHOsoil} \qquad \textbf{(411)}$$

$$Clocal_{soil} = Clocal\_soil_{direct} + Clocal\_soil_{indirect} \qquad \textbf{(412)}$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_{contr}$	[d]	21

Input

Qprod	amount of product used at each refilling	[kg]	S
Nsites	number of application sites	[-]	D
Nrefill	number of refilling times	[-]	D
Fsubst	fraction of active substance in product	[$kg_c.kg^{-1}$]	S
$Fdirect_{soil}$	fraction of active substance release directly to soil	[-]	D
$AREA_{expo,direct}$	area around one box directly exposed to active substance	[m^2]	D
$AREA_{expo,indirect}$	area indirectly exposed to active substance	[m^2]	D
DEPTHsoil	depth of exposed soil	[m]	D
RHOsoil	density of wet soil	[$kg_{wwt}.m^{-3}$]	D
$Temission_{contr}$	number of emission days during the control operation	[d]	D/S
Fmetab	fraction of active ingredient metabolised	[-]	D/S
$Fexcr_{soil}$	fraction of substance released indirectly to soil via excretion	[-]	O
$Clocal\_soil_{direct}$	local concentration in soil due to direct release after campaign	[$kg_c.kg_{wwt}^{-1}$]	O
$Clocal\_soil_{indrect}$	local concentration in soil due to indirect release after campaign	[$kg_c.kg_{wwt}^{-1}$]	O

Output

$Clocal_{soil}$	local concentration in soil	[$kg_c.kg_{wwt}^{-1}$]	O
Temission	number of emission days	[d]	O

Table III-113 Default settings of the model for bait boxes used for control around buildings.

Parameter	**Symbol**	**Unit**	**Value**
Amount of product used at each refilling	Qprod	[kg]	-
Fraction of active substance in product	Fsubst	[$kg_c.kg^{-1}$]	-
Number of application sites	Nsites	[-]	10
Number of refilling times	Nrefill	[-]	5
Fraction of active substance released directly to soil	$Fdirect_{soil}$	[-]	0.01
Area around one box directly exposed to active substance	$AREA_{expo,direct}$	[m^2]	0.09
Area indirectly exposed to active substance	$AREA_{expo,indirect}$	[m^2]	550
Depth of exposed soil	DEPTHsoil	[m]	0.1
density of wet soil	RHOsoil	[$kg_{wwt}.m^{-3}$]	1700
Number of emission days for control operation	$Temission_{contr}$	[d]	21
Fraction of active substance metabolised	Fmetab	[-]	0

Parameters/variables and default values for release through use of liquid concentrates.

Direct release

$$Clocal\_soil_{direct} = \frac{Qprod \cdot Fsubst \cdot Nsites \cdot Nrefill \cdot (Fappl_{soil} + Fuse_{soil})}{AREA_{expo,direct} \cdot DEPTsoil \cdot RHOsoil \cdot Nsites} \tag{413}$$

Indirect release (via excretion)

$$Fexcr_{soil} = 0.3 + (0.6 - Fmetab) \tag{414}$$

$$Clocal\_soil_{indirect} = \frac{Qprod \cdot Fsubst \cdot Nsites \cdot Nrefill \cdot Fexcr_{soil} \cdot (1 - Fappl_{soil} - Fuse_{soil})}{AREA_{expo,indirect} \cdot DEPTHsoil \cdot RHOsoil} \tag{415}$$

$$Clocal_{soil} = Clocal\_soil_{direct} + Clocal\_soil_{indirect} \tag{416}$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_{contr}$	[d]	21

Input

Qprod	amount of product used at each refilling	[kg]	S
Nsites	number of application sites	[-]	D
Nrefill	number of refilling times	[-]	D
Fsubst	fraction of active substance in product	$[kg_c.kg^{-1}]$	S
$Fuse_{soil}$	fraction of active substance released to soil during use	[-]	D
$Fappl_{soil}$	fraction of active substance released to soil from the application	[-]	D
$AREA_{expo,direct}$	area directly exposed to active substance	$[m^2]$	D
$AREA_{expo,indirect}$	area indirectly exposed to active substance	$[m^2]$	D
DEPTHsoil	depth of exposed soil	[m]	D
RHOsoil	density of wet soil	$[kg_{wwt}.m^{-3}]$	D
$Temission_{contr}$	number of emission days during the control operation	[d]	D/S
Fmetab	fraction of active ingredient metabolised	[-]	D/S
$Fexcr_{soil}$	fraction of substance released indirectly through excretion	[d]	O
$Clocal\_soil_{direct}$	local concentration in soil due to direct release after campaign	$[kg_c.kg_{wwt}^{-1}]$	O
$Clocal\_soil_{indrect}$	local concentration in soil due to indirect release after campaign	$[kg_c.kg_{wwt}^{-1}]$	O

Output

$Clocal_{soil}$	local concentration in soil	$[kg_c.kg_{wwt}^{-1}]$	O
Temission	number of emission days	[d]	O

Table III-114 Default settings of the model for the use of liquid concentrates in control around buildings.

Parameter	Symbol	Unit	Value
Amount of product used at each refilling	Qprod	[kg]	-
Fraction of active substance in product	Fsubst	$[kg_c.kg^{-1}]$	-
Number of application sites	Nsites	[-]	10
Number of refilling times	Nrefill	[-]	5
Fraction of active substance released to soil during use	$Fuse_{soil}$	[-]	0.10
Fraction of active substance release to soil during application	$Fappl_{soil}$	[-]	0.05
Area directly exposed to active substance	$AREA_{expo,direct}$	$[m^2]$	0.0314
Area indirectly exposed to active substance	$AREA_{expo,indirect}$	$[m^2]$	550
Depth of exposed soil	DEPTHsoil	[m]	0.1
density of wet soil	RHOsoil	$[kg_{wwt}.m^{-3}]$	1700
Number of emission days for control operation	$Temission_{contr}$	[d]	21
Fraction of active substance metabolised	Fmetab	[-]	0

III.3.6.12.3 Products used for control in open areas

Parameters/variables and default values for release through use of pellets and impregnated grain.

$$Vsoil = \frac{(R^2 - r^2) \cdot \pi \cdot l}{2} \tag{417}$$

$$Clocal_{soil} = \frac{Qprod \cdot Fsubst \cdot Nsites \cdot Nrefill \cdot (Fappl_{soil} + Fuse_{soil})}{Vsoil \cdot RHOsoil} \tag{418}$$

Parameters required for distribution modules	Defaults for this scenario	Unit	Value
Temission	$Temission_{contr}$	[d]	6

Input			
R	radius of exposed soil around hole	[m]	D
r	radius of the hole	[m]	D
l	length of exposed hole	[m]	D
Qprod	amount of product used at each refilling	[kg]	S
Nsites	number of application sites	[-]	D
Nrefill	number of refilling times	[-]	D
Fsubst	fraction of active substance in product	$[kg_c.kg^{-1}]$	S
$Fuse_{soil}$	fraction of active substance released to soil during use	[-]	D
$Fappl_{soil}$	fraction of active substance released to soil during application	[-]	D
RHOsoil	density of wet soil	$[kg_{wwt}.m^{-3}]$	D
Vsoil	volume of exposed soil	$[m^3]$	O
$Temission_{contr}$	number of emission days during the control operation	[d]	D
Output			
$Clocal_{3,soil}$	local concentration in soil	$[kg_c.kg_{wwt}^{-1}]$	O
Temission	number of emission days	[d]	O

Table III-115 Default settings of the model for control in open areas with impregnated grain.

Parameter	**Symbol**	**Unit**	**Value**
Amount of product used at each refilling	Qprod	[kg]	-
Fraction of active substance in product	Fsubst	$[kg_c.kg^{-1}]$	-
Number of application sites	Nsites	[-]	1
Number of refilling times	Nrefill	[-]	2
Fraction of active substance released to soil during use	$Fuse_{soil}$	[-]	0.20
Fraction of active substance release to soil during application	$Fappl_{soil}$	[-]	0.05
Radius of exposed soil around the hole	R	[m]	0.14
Radius of the hole	r	[m]	0.04
Length of exposed hole	l	[m]	0.3
density of wet soil	RHOsoil	$[kg_{wwt}.m^{-3}]$	1700
Number of emission days for control operation	$Temission_{contr}$	[d]	6

Parameters/variables and default values for release through use of contact powder.

$$Vsoil = \frac{(R^2 - r^2) \cdot \pi \cdot l}{2} \qquad \textbf{(419)}$$

$$Clocal_{3,soil} = \frac{Qprod \cdot Fsubst \cdot Nsites \cdot F_{3,soil}}{Vsoil \cdot RHOsoil} \qquad \textbf{(420)}$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_{contr}$	[d]	1

Input

R	radius of exposed soil around hole	[m]	D
r	radius of the hole	[m]	D
l	length of exposed hole	[m]	D
Qprod	amount of product used at each refilling	[kg]	S
Nsites	number of application sites	[-]	D
Fsubst	fraction of active substance in product	$[kg_c.kg^{-1}]$	S
$F_{3,soil}$	fraction of active substance released to soil	[-]	D
RHOsoil	density of wet soil	$[kg_{wwt}.m^{-3}]$	D
Vsoil	volume of exposed soil	$[m^3]$	O
$Temission_{contr}$	number of emission days during the control operation	[d]	D

Output

$Clocal_{3,soil}$	local concentration in soil	$[kg_c.kg_{wwt}^{-1}]$	O
Temission	number of emission days	[d]	O

Table III-116 Default settings of the model for control in open areas with contact powder.

Parameter	**Symbol**	**Unit**	**Value**
Amount of product used at each refilling	Qprod	[kg]	-
Fraction of active substance in product	Fsubst	$[kg_c.kg^{-1}]$	-
Number of application sites	Nsites	[-]	1
Fraction of active substance released to soil	$F_{3,soil}$	[-]	0.9
Radius of exposed soil around the hole	R	[m]	0.14
Radius of the hole	r	[m]	0.04
Length of exposed hole	l	[m]	0.3
density of wet soil	RHOsoil	$[kg_{wwt}.m^{-3}]$	1700
Number of emission days for control operation	$Temission_{contr}$	[d]	1

Parameters/variables and default values for release through gassing.

$$Vsoil \ = (R^2 - r^2) \cdot \pi \cdot l \qquad \textbf{(421)}$$

$$Clocal_{soil} = \frac{Qprod \cdot Fsubst \cdot Fformed \cdot Nappl \cdot F_{3,soil}}{\cdot Vsoil \cdot RHOsoil} \qquad \textbf{(422)}$$

$$DOSEprod = \frac{Qprod}{AREA_{contr}} \qquad \textbf{(423)}$$

$$Clocal_{air} = \frac{DOSEprod \cdot Fsubst \cdot Fformed \cdot (1 - F_{3,soil}) \cdot Estd_{field,air,24h}}{HEIGHTair} \qquad \textbf{(424)}$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	Temission$_{contr}$	[d]	1

Input

-	type of product used	[-]	P
R	radius of exposed soil around hole	[m]	D
r	radius of the hole	[m]	D
l	length of exposed hole	[m]	D
Qprod	amount of product used per 2 ha in control operation	[kg]	S
AREA$_{contr}$	area treated at control operation	[m^2]	D
DOSEprod	amount of product used per unit of treated area	[kg.m^{-2}]	O
Nappl	number of applications	[-]	D
Fsubst	fraction of substance in product	[kg$_c$.kg^{-1}]	S
Fformed	fraction of phosphine formed	[-]	O^c
F$_{3,soil}$	fraction of active substance released to soil	[-]	D
RHOsoil	density of wet soil	[kg$_{wwt}$.m^{-3}]	D
Vsoil	volume of exposed soil per treated area (2 ha)	[m^3]	O
HEIGHTair	atmospheric mixing height	[m]	D
Estd$_{field,air,24h}$	24 hour average source strength	[-]	D
Temission$_{cont}$	number of emission days during the control operation	[d]	D

Output

Clocal$_{3,soil}$	local concentration in soil from an application	[kg$_c$.kg$_{wwt}$$^{-1}$]	O
Clocal$_{3,air}$	local concentration in air from an application	[kg$_c$.m^{-3}]	O
Temission	number of emission days	[d]	O

Table III-117 Default settings of the model for control in open areas through gassing.

Parameter	**Symbol**	**Unit**	**Value**
Amount of product used per 2 ha in control operation	Qprod	[kg]	-
Area treated at control operation	$AREA_{contr}$	[m^2]	20 000
Fraction of substance (metal phosphide) in product	Fsubst	[$kg_c.kg^{-1}$]	-
Fraction of active substance (phosphine) formed	Fformed	[-]	
Aluminium phosphide			0.586
Magnesium phosphide			0.504
Zinc phosphide			0.263
Number of applications	Nappl	[-]	1
Fraction of active substance released to soil	$F_{3,soil}$	[-]	0.99
Radius of exposed soil around the hole	R	[m]	0.14
Radius of the hole	r	[m]	0.04
Length of exposed hole	l	[m]	1000
24 hour average source strength	$Estd_{field, air, 24 h}$	[-]	0.9*
Atmospheric mixing height	HEIGHTair	[m]	2
density of wet soil	RHOsoil	[$kg_{wwt}.m^{-3}$]	1700
Number of emission days for control operation	$Temission_{cont}$	[d]	1

* 24 hour average source strength has a value of 0.9 for all substance with a vapour pressure > 0.01 Pa

III.3.6.12.4 Products used for rodent control at waste dumps and landfills

Parameters/variables and default values for release at waste dumps through use of bait boxes and or wax blocks.

$$Clocal_{3,soil} = \frac{Qprod \cdot Fsubst \cdot Nappl \cdot F_{3,soil}}{AREAexpo \cdot DEPTHsoil \cdot RHOsoil} \qquad \textbf{(425)}$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_{contr}$	[d]	365

Input			
Qprod	amount of product used at each refilling	[kg]	S/D
Nappl	number of applications	[-]	D/S
Fsubst	fraction of active substance in product	$[kg_c.kg^{-1}]$	S
$F_{3,soil}$	fraction of active substance released to soil	[-]	D/S
RHOsoil	density of wet soil	$[kg_{wwt}.m^{-3}]$	D
$Temission_{contr}$	number of emission days during the control operation	[d]	D
Output			
$Clocal_{soil}$	local concentration in soil	$[kg_c.kg_{wwt}^{-1}]$	O
Temission	number of emission days	[d]	O

Table III-118 Default settings of the model for control at waste dumps and landfills.

Parameter	**Symbol**	**Unit**	**Value**
Amount of product used at each refilling	Qprod	[kg]	40
Number of applications	Nappl	[-]	7
Fraction of active substance released to soil	$Frelease_{soil}$	[-]	0.9
Fraction of active substance release to soil during application	$Fappl_{soil}$	[-]	0.05
Area exposed to rodenticide	AREAexpo	$[m^2]$	10 000
Depth of exposed soil	DEPTHsoil	[m]	0.10
Density of wet soil	RHOsoil	$[kg_{wwt}.m^{-3}]$	1700
Number of emission days for control operation	$Temission_{contr}$	[d]	365

III.3.6.12.5 Primary and secondary poisoning for rodenticides

For the prediction of primary and secondary poisoning, the daily mean food intake is needed. For a number of birds default body weights and daily mean food intakes are given in the ESD (see ***Table III-120***). If no information is available, the regression equations presented below can be used to predict dry weight intake for an animal of a particular body weight (see ***Table III-120***). The list of birds and mammals with only the default values for the body weight is taken from RIVM, VROM, VWS (2002).

Parameters/variables and default values for primary poisoning.

$$C_{food} = Fsubst \tag{426}$$

$$RCR_{bird,mammal} = \frac{C_{food}}{NOEC_{bird,mammal}} \tag{427}$$

if C_{food}>$NOEC_{bird}$ or $NOEC_{mammal,food,\ chr}$, then

all birds

$$\log DFI_{bird} = 0.651 \cdot \log BW_{bird} - 0.188 \tag{428}$$

song birds

$$\log DFI_{bird} = 0.850 \cdot \log BW_{bird} - 0.400 \tag{429}$$

non songs birds

$$\log DFI_{bird} = 0.751 \cdot \log BW_{bird} - 0.521 \tag{430}$$

mammals

$$\log DFI_{mammal} = 0.822 \cdot \log BW_{mammal} - 0.629 \tag{431}$$

$$ETE_{bird\,/\,mammal} = \frac{DFI_{bird\,/\,mammal} \cdot C_{food} \cdot AV \cdot PT \cdot PD}{BW_{bird\,/\,mammal}} \tag{432}$$

Input			
-	bird species of concern	[-]	P
-	mammalian species of concern	[-]	P
Fsubst	fraction of active substance in product	$[kg_c.kg^{-1}]$	S
C_{food}	concentration in food	$[kg_c.kg_{food}^{-1}]$	S/O
$DFI_{bird/mammal}$	daily food intake rate of indicator species	$[kg_{food}.d^{-1}]$	S/O
$BW_{bird/mammal}$	body weight of indicator species	$[kg_{BW}]$	S/O
AV	avoidance factor	[-]	S/D
PT	fraction of diet obtained in treated area	[-]	S/D
PD	fraction of food type in diet	[-]	S/D
$ETE_{bird/mammal}$	estimated daily uptake of a compound by indicator species	$[kg_c.kg_{BW}^{-1}.d^{-1}]$	O
$NOEC_{bird,mammal}$	NOEC for birds or mammals	$[kgc.kg_{food}^{-1}.d^{-1}]$	S
$NOAEL_{bird/mammal}$	NOAEL for birds or mammals	$[kg_c.kg_{BW}^{-1}.d^{-1}]$	S
Output			
$RCR_{bird/mammal}$	risk characterisation ratio for indicator species	[-]	O

Table III-119 Default settings of the model for primary poisoning.

Parameter	**Symbol**	**Unit**	**Value**
Fraction of active substance in product	Fsubst	[-]	-
Daily food intake rate of indicator species	DFI	[$kg_{food}.d^{-1}$]	equation 435-438
Body weight of indicator species	BW	[kg_{BW}]	***Table III-120***
Avoidance factor (1= no avoidance, 0 = complete avoidance)	AV	[-]	1
Fraction of diet obtained in treated area (value between 0 and 1)	PT	[-]	1
Fraction of food type in diet (number between 0 and 1; on or more types)	PD	[-]	1

Table III-120 Default body weight for target species for primary poisoning from RIVM (2002).

Species	**Mean body weight**	**Daily food intake**
Birds		
Default	10	
Quail	102	
Common Partridge	375	
Common Pheasant	953	102.7
Turtle Dove	152	
Collared Dove	195	
Wood pigeon	440	53.1
Feral pigeon	360	41.4
Chaffinch	22	6.4
Goldfinch	15	
Common Redpoll	14	
House sparrow	27	9
Tree sparrow	22	7.6
Mammals		
Wild mammals		
Default (Pygmy shrew)	6	
Hedgehog	700	
Mole	100	
Woodshrew	9.5	
Hare	4500	
Rabbit	1900	
Field mouse	27	
Wood mouse	24.5	
Brown rat	370	
Badger	11 250	
Domestic mammals		
Dog	10 000	
Pig (young)	25 000	maximum 600
Hog	80 000	maximum 600

Parameters/variables and default values for secondary poisoning.

$$C_{food} = Fsubst \qquad \textbf{(433)}$$

mammals

$$ETE_{rodent} = \frac{DFI_{rodent} \cdot C_{food} \cdot AV \cdot PT \cdot PD}{BW_{rodent}} \qquad \textbf{(434)}$$

$$IRC_{rodent} = \sum_{n=1}^{Ndays} ETE_{rodent} \cdot (1 - Felim_{rodent})^{n} \qquad \textbf{(435)}$$

$$PEC_{oral,predator} = \left(IRC_{rodent,Ndays} + ETE_{rodent}\right) \cdot F_{rodent} \qquad \textbf{(436)}$$

$$RCR_{predator} = \frac{PEC_{oral,predator}}{PNEC_{oral,predator}} \qquad \textbf{(437)}$$

Input			
-	mammalian species of concern	[-]	P
Fsubst	fraction of active substance in product	$[kg_c.kg^{-1}]$	S
C_{food}	concentration in food	$[kg_c.kg_{food}^{-1}]$	S/O
DFI_{mammal}	daily food intake rate of target species	$[kg_{food}.d^{-1}]$	S/O
BW_{mammal}	body weight of target species	$[kg_{BW}]$	S/O
AV	avoidance factor	[-]	S/D
PT	fraction of diet obtained in treated area	[-]	S/D
PD	fraction of food type in diet	[-]	S/D
Felim	elimination of the active substance	[-]	S/D
Ndays	number of days the rodent is eating rodenticide before it is caught by the predator	[-]	S/D
ETE_{rodent}	estimated uptake of a compound by rodent	$[kg_c.kg_{BW}^{-1}.d^{-1}]$	O^c
IRC_{rodent}	internal residual concentration in rodent before last meal	$[kg_c.kg_{BW}^{-1}]$	O^c
$PEC_{oral,\ predator}$	concentration in food of predator	$[kg_c.kg_{food}^{-1}]$	O^c
F_{rodent}	fraction of poisoned rodents in predator’s diet	[-]	D
$PNEC_{oral,predator}$	NOEC for predators	$[kg_c.kg_{food}^{-1}]$	S
Output			
$RCR_{predator}$	risk characterisation ratio for predator	[-]	O

Table III-121 Default settings of the model for secondary poisoning.

Parameter	**Symbol**	**Unit**	**Value**
Fraction of active substance in product	Fsubst	[-]	-
Daily food intake rate of indicator species	DFI	[$kg_{food}.d^{-1}$]	equation 435-438
Body weight of indicator species	BW	[kg_{BW}]	***Table III-120***
Avoidance factor (1= no avoidance, 0 = complete avoidance)	AV	[-]	1
Fraction of diet obtained in treated area (value between 0 and 1)	PT	[-]	1
Fraction of food type in diet (number between 0 and 1; on or more types)	PD	[-]	1
Elimination of active substance	Felim	[-]	0.3
Number of days the rodent is eating rodenticide before it is caught by the predator	N_{days}	[-]	5
Fraction of poisoned rodents in predator's diet	F_{rodent}		
short term			1
long term			0.5

III.3.6.13 Product type 15: Avicides

The scenarios, models and calculation used in this version of EUSES 2.1.1 for avicides have been taken from the following document:

- Supplement to the methodology for risk evaluation of biocides, Emission Scenarios for biocides used as avicides (Product type 15) (EUBEES, 2003).

This document can be obtained from the ECB Biocides website

The following addition is made:
In the ESD no method is given to determine the risk characterisation ratio (RCR) for secondairy poisoning. This formula has been added. For primairy poisoning no RCR is determined.

III.3.6.13.1 Bird control management using baits in the open area

Parameters/variables and default values for bait preparation, life cycle stage formulation.

Feral pigeons

$$Elocal_{2,water} = \frac{Nappl \cdot Nbird \cdot Nflocks \cdot Qbird \cdot Fsubst \cdot F_{2,water}}{Temission_{prep}} \qquad \textbf{(438)}$$

House sparrow

$$Elocal_{2,water} = \frac{Nappl \cdot Nsites \cdot \; Qsite \cdot Fsubst \cdot F_{2,water}}{Temission_{prep}} \qquad \textbf{(439)}$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_{prep}$	[d]	1

Input			
Nappl	number of applications	[-]	D
Nbird	number of birds in a flock	[-]	D
Nflocks	number of flocks	[-]	D
Qbird	amount of bait used per bird	[kg]	D
Nsites	number of feeding points	[-]	D
Qsite	amount of product used per site	[-]	D
Fsubst	fraction of active substance in product (bait)	$[kg_c.kg^{-1}]$	S
$F_{2,water}$	fraction of product released to waste water	[-]	D
$Temission_{prep}$	number of emission days for bait preparation	[d]	D
Output			
Temission	number of emission days	[d]	O
$Elocal_{2,water}$	local emission of to waste water during episode	$[kg_c.d^{-1}]$	O

Table III-122 Default settings of the model for bait preparation.

Parameter	**Symbol**	**Unit**	**Value**
Number of applications Feral pigeons House sparrows	Nappl	[-]	 3 6
Number of birds in a flock	Nbird	[-]	150
Number of flocks	Nflocks	[-]	1
Amount of bait used per bird	Qbird	[kg]	0.05
Number of feeding points	Nsites	[-]	30
Amount of product used per site	Qsite	[kg]	0.05
Fraction of active substance in product (bait)	Fsubst	$[kg_c.kg^{-1}]$	-
Fraction of active substance released to waste water	$F_{2.water}$	[-]	0.05
Number of emission days for bait preparation	$Temission_{prep}$	[d]	1

Parameters/variables and default values for bait application, life cycle stage professional use.

Feral pigeons

$$Elocal_{3,soil} = Nappl \cdot Nbird \cdot Nflocks \cdot Qbird \cdot Fsubst \cdot F_{3,soil} \quad \textbf{(440)}$$

$$Clocal_{soil} = \frac{Elocal_{3,soil}}{AREAsite \cdot Nflocks \cdot DEPTHsoil \cdot RHOsoil} \quad \textbf{(441)}$$

House sparrow

$$Elocal_{3,soil} = Nappl \cdot Nsites \cdot Qsite \cdot Fsubst \cdot F_{3,soil} \quad \textbf{(442)}$$

$$Clocal_{soil} = \frac{Elocal_{3,soil}}{AREAsite \cdot Nsites \cdot DEPTHsoil \cdot RHOsoil} \quad \textbf{(443)}$$

Input

-	Type of feed used for house sparrow	[-]	P
Nappl	number of applications	[-]	D/O
Nbird	number of birds in a flock	[-]	D
Nflocks	number of flocks	[-]	D
Qbird	amount of bait used per bird	[kg]	D
Nsites	number of feeding points	[-]	D
Qsite	amount of product used per site	[-]	D
Fsubst	fraction of active substance in product (bait)	[$kg_c.kg^{-1}$]	S
AREAsite	surface area of site	[m^2]	D
RHOsoil	density of wet soil	[$kg_{wwt}.m^{-3}$]	D
DEPTHsoil	depth of soil	[m]	D
$Elocal_{3,soil}$	local emission of active substance to soil	[kg]	O^c
Output			
$Clocal_{soil}$	local emission of active substance to soil	[$kg_c.kg_{wwt}$]	O

Table III-123 Default settings of the model for bait application.

Parameter	**Symbol**	**Unit**	**Value**
Number of applications	Nappl	[-]	
Feral pigeons			3
House sparrows			
- grain			2
- bread			6
Number of birds in a flock	Nbird	[-]	150
Number of flocks	Nflocks	[-]	1
Amount of bait used per bird	Qbird	[kg]	0.05
Number of feeding points	Nsites	[-]	30
Amount of product used per site	Qsite	[kg]	0.05
Fraction of active substance in product (bait)	Fsubst	[$kg_c.kg^{-1}$]	-
Fraction of active substance released to soil	$F_{3,soil}$	[-]	0.80
Site area directly exposed to avicide	AREAsite	[m^2]	
Feral pigeons			12.5
House sparrow			0.1
Depth of exposed soil	DEPTHsoil	[m]	0.1
Density of wet soil	RHOsoil	[$kg_{wwt}.m^{-3}$]	1700

III.3.6.13.2 Bird control management in the open area using egg-oil coating

Parameters/variables and default values for application of egg-oil coating.

$$Elocal_{3,soil} = Nnest \cdot Neggs \cdot Vform_{egg} \cdot RHOform \cdot Fsubst \cdot Nappl \cdot F_{3,soil} \qquad \textbf{(444)}$$

$$Clocal_{soil} = \frac{Elocal_{3,soil}}{AREAsoil \cdot Nnest \cdot Nappl \cdot DEPTHsoil \cdot RHOsoil} \qquad \textbf{(445)}$$

Input

-	type of application	[-]	P
Nnest	number of nests to be treated at one site	[-]	D
Negg	number of eggs per nest	[-]	D
Nappl	number of applications	[-]	D
$Vform_{egg}$	amount of product needed to cover one egg completely	[m^3]	D
Fsubst	fraction of active substance in product	[$kg_c.kg^{-1}$]	S
RHOform	density of product	[$kg.m^{-3}$]	S
$F_{3.soil}$	fraction of product lost during application	[-]	O
AREAsoil	surface area near nest	[m^2]	D
RHOsoil	density of wet soil	[$kg_{wwt}.m^{-3}$]	D
DEPTHsoil	depth of soil	[m]	D
$Elocal_{3,soil}$	local emission of active substance to soil during campaign	[kg]	O^c
Output			
$Clocal_{soil}$	local concentration of active substance in soil	[$kg_c.kg_{wwt}$]	O

Table III-124 Default settings of the model for egg-oil application.

Parameter	Symbol	Unit	Value
Number of nests to be treated at one site	Nnest	[-]	150
Number of eggs per nest	Negg	[-]	6
Number of applications	Nappl	[-]	1
Volume of product needed to cover one egg completely	$Vform_{egg}$	[m^3]	7.10^{-6}
Fraction of active substance in product	Fsubst	[$kg_c.kg^{-1}$]	-
Fraction of active substance released to soil spraying immersion	$F_{3.soil}$	[-]	 0.1 0.0
Density of product	RHOform	[$kg_{wwt}.m^{-3}$]	-
Exposed area near nest (nest+surrounding surface)	AREAsoil	[m^2]	0.33
Depth of exposed soil	DEPTHsoil	[m]	0.1
Density of wet soil	RHOsoil	[$kg.m^{-3}$]	1700

Parameters/variables and default values for release of egg-oil during service life (life cycle stage 5).

$$Qleach = Neggs \cdot Vform_{egg} \cdot RHOform \cdot Fsubst \cdot Nappl \cdot (1 - F_{3,soil} - Fdrift) \qquad \textbf{(446)}$$

$$Elocal_{5,soil} = Qleach \cdot \sum_{i=1}^{Nrain} Fleach \cdot (1 - Fleach)^{Nrain-1} \qquad \textbf{(447)}$$

$$Clocal_{soil} = \frac{Elocal_{5,soil}}{AREAsoil \cdot Nappl \cdot DEPTHsoil \cdot RHOsoil} + Clocal_{appl,soil} \qquad \textbf{(448)}$$

Input			
-	type of application	[-]	P
Negg	number of eggs per nest	[-]	D
Nappl	number of applications	[-]	D
Vform$_{egg}$	amount of product needed to cover one egg completely	[m^3]	D
Fsubst	fraction of active substance in product	[kg$_c$.kg^{-1}]	S
RHOform	density of product	[kg.m^{-3}]	S
F$_{3.soil}$	fraction of product lost to soil during application	[-]	O
Fdrift	fraction of product lost during application due to spray-drift	[-]	D
Nrain	number of rain events	[-]	D
Fleach	fraction of product lost during application due to spray-drift	[-]	D
Qleach	quantity of active substance on egg just after the application	[kg]	O
Elocal$_{5,soil}$	local emission of active substance to soil due to leaching	[-]	O^c
AREAsoil	surface area near nest	[m^2]	D
RHOsoil	density of wet soil	[kg$_{wwt}$.m^{-3}]	D
DEPTHsoil	depth of soil	[m]	D
Clocal$_{appl,soil}$	local concentration in soil due to application (stage 3)	[kg$_c$.kg$_{wwt}$$^{-1}$]	O^c
Output			
Clocal$_{soil}$	total local emission of active substance to soil	[kg$_c$.kg$_{wwt}$$^{-1}$]	O

Table III-125 Default settings of the model for release of egg-oil during service life.

Parameter	**Symbol**	**Unit**	**Value**
Number of eggs per nest	Negg	[-]	6
Number of applications	Nappl	[-]	1
Volume of product needed to cover one egg completely	$Vform_{egg}$	[m^3]	7.10^{-6}
Fraction of active substance in product	Fsubst	[$kg_c.kg^{-1}$]	-
Fraction of product released to soil during application spraying immersion	$F_{3.soil}$	[-]	 0.1 0.0
Fraction of used product lost due to spray-drift	Fdrift	[-]	0.1
Fraction of product released by leaching	Fleach	[-]	0.1
Number of rain events	Nrain	[-]	11
Density of product	RHOform	[$kg.m^{-3}$]	-
Exposed area near nest (nest+surrounding surface)	AREAsoil	[m^2]	0.33
Depth of exposed soil	DEPTHsoil	[m]	0.1
Density of wet soil	RHOsoil	[$kg.m^{-3}$]	1700

III.3.6.13.3 Bird control management in and around buildings through bait application

Parameters/variables and default values for bait application.

Feral pigeons

$$Elocal_{3,water} = \frac{Nappl \cdot Nbird \cdot Nflocks \cdot Qbird \cdot Fsubst \cdot F_{3,water}}{Temission_{contr}} \tag{449}$$

House sparrow

$$Elocal_{3,water} = \frac{Nappl \cdot Nsites \cdot \; Qsite \cdot Fsubst \cdot F_{3,water}}{Temission_{contr}} \tag{450}$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_{contr,pigeon}$	[d]	5
Temission	$Temission_{contr,sparrouw}$	[d]	2

Input

-	type of bait used	[-]	P
Nappl	number of applications	[-]	D/O
Nbird	number of birds in a flock	[-]	D
Nflocks	number of flocks	[-]	D
Qbird	amount of bait used per bird	[kg]	D
Nsites	number of feeding points	[-]	D
Qsite	amount of product used per site	[-]	D
Fsubst	fraction of active substance in product (bait)	$[kg_c kg^{-1}]$	S
$Temission_{contr}$	number of emission days for control campaign	[d]	D
Output			
Temission	number of emission days	[d]	O
$Elocal_{3,water}$	local emission of to waste water during episode	$[kg_c.d^{-1}]$	O

Table III-126 Default settings of the model for bait application.

Parameter	Symbol	Unit	Value
Number of applications	Nappl	[-]	
Feral pigeons			3
House sparrows			
- grain			2
- bread			6
Number of birds in a flock	Nbird	[-]	150
Number of flocks	Nflocks	[-]	1
Amount of bait used per bird	Qbird	[kg]	0.05
Number of feeding points	Nsites	[-]	30
Amount of product used per site	Qsite	[kg]	0.05
Fraction of active substance in product (bait)	Fsubst	[-]	-
Fraction of active substance released to waste water	$F_{3.water}$	[-]	0.70
Number of emission days for a control campaign	$Temission_{contr}$	[d]	
Feral pigeons			5
House sparrow			2

III.3.6.13.4 Bird control management in and around buildings using egg-oil coating

Parameters/variables and default values for application of egg-oil coating.

$$Quse = Nsites \cdot Nnest \cdot Neggs \cdot Vform_{egg} \cdot RHOform \cdot Fsubst \cdot Nappl \tag{451}$$

$$Elocal_{drift} = \frac{Quse \cdot Fdrift}{Temission_{appl}} \tag{452}$$

$$Elocal_{leach} = \frac{Quse \cdot (1 - Fdrift) \cdot Fleach}{Temission_{leach}} \tag{453}$$

$$Elocal_{3,water} = Elocal_{drift} + Elocal_{leach} \tag{454}$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	Temission$_{leach}$	[d]	1

Input			
-	controlled species	[-]	P
Nsites	number of application sites	[-]	D
Nnest	number of nests to be treated at one site	[-]	D
Negg	number of eggs per nest	[-]	D
Nappl	number of applications	[-]	D
Vform$_{egg}$	amount of product needed to cover one egg completely	[m^3]	D
Fsubst	fraction of active substance in product	[kg$_c$.kg]	S
RHOform	density of product	[kg.m^{-3}]	S
Fdrift	fraction of product lost during application	[-]	D
Fleach	fraction of product lost due to leaching after rain event	[-]	D
Quse	amount of substance used for eggs-coating	[kg$_c$]	O
Elocal$_{drift}$	local emission of active substance to water due to drift	[-]	O
Elocal$_{drift}$	local emission of active substance to water due to leaching	[-]	O
Temission$_{leach}$	number of emission days for leaching at the stage of service life	[d]	D
Temission$_{appl}$	number of emission days for the stage of application	[d]	D
Output			
Temission	number of emission days	[-]	O
Elocal$_{3,water}$	local emission of active substance to waste water	[kg$_c$.d^{-1}]	O

Table III-127 Default settings of the model for egg-oil application.

Parameter	**Symbol**	**Unit**	**Value**
Number of application sites	Nsites	[-]	1
Number of nests to be treated at one site	Nnest	[-]	1000
Number of eggs per nest	Negg	[-]	3
Number of applications	Nappl	[-]	1
Volume of product needed to cover one egg completely	$Vform_{egg}$	[m^3]	
Lesser Black-backed Gull			$2.6.10^{-6}$
Herring Gull			$2.9.10^{-6}$
Great Black-backed Gull			$3.4.10^{-6}$
Fraction of active substance released to waste water due to spraying	Fdrift	[-]	0.1
Fraction of active substance released to waste water due to leaching	Fleach	[-]	0.1
Density of product	RHOform	[$kg.m^{-3}$]	-
Number of emission days for the stage of application	$Temission_{appl}$	[d]	2
Number of emission days for the stage of service life	$Temission_{leach}$	[d]	1

III.3.6.13.5 Primary and secondary poisoning for avicides

For the prediction of primary and secondary poisoning, the daily mean food intake is needed. For a number of birds default body weights and daily mean food intakes are given in the ESD (see *Table III-120*). If no information is available, the regression equations presented below can be used to predict dry weight intake for an animal of a particular body weight (see *Table III-120*). The list of birds and mammals with only the default values for the body weight is taken from RIVM, VROM, VWS (2002).

Parameters/variables and default values for primary poisoning.

$$C_{food} = Fsubst \tag{455}$$

$$RCR_{bird,mammal} = \frac{C_{food}}{NOEC_{bird,mammal}} \tag{456}$$

if C_{food}>$NOEC_{bird}$ or $NOEC_{mammal,food,\ chr}$, then

all birds

$$\log(DFI_{bird} \cdot 1000) = 0.651 \cdot \log(BW_{bird} \cdot 1000) - 0.188 \tag{457}$$

songbirds

$$\log(DFI_{bird} \cdot 1000) = 0.850 \cdot \log(BW_{bird} \cdot 1000) - 0.400 \tag{458}$$

non songbirds

$$\log(DFI_{bird} \cdot 1000) = 0.751 \cdot \log(BW_{bird} \cdot 1000) - 0.521 \tag{459}$$

mammals

$$\log(DFI_{mammal} \cdot 1000) = 0.822 \cdot \log(BW_{mammal} \cdot 1000) - 0.629 \tag{460}$$

$$ETE_{bird\,/\,mammal} = \frac{DFI_{bird\,/\,mammal} \cdot C_{food} \cdot AV \cdot PT \cdot PD}{BW_{bird\,/\,mammal}} \tag{461}$$

Input

-	bird species of concern	[-]	P
-	mammalian species of concern	[-]	P
Fsubst	fraction of active substance in product	[-]	S
C_{food}	concentration in food	$[kg_c.kg_{food}^{-1}]$	S/O
$DFI_{bird/mammal}$	daily food intake rate of indicator species	$[kg_{food}.d^{-1}]$	S/O
$BW_{bird/mammal}$	body weight of indicator species	$[kg_{BW}]$	S/O
AV	avoidance factor	[-]	S/D
PT	fraction of diet obtained in treated area	[-]	S/D
PD	fraction of food type in diet	[-]	S/D
$ETE_{bird/mammal}$	estimated daily uptake of a compound by indicator species	$[kg_c.kg_{BW}^{-1}.d^{-1}]$	O
$NOEC_{bird,mammal}$	NOEC for bird or mammal of concern	$[kg_c.kg_{food}^{-1}.d^{-1}]$	S
$NOAEL_{bird/mammal}$	NOAEL for bird or mammal of concern	$[kg_c.kg_{BW}^{-1}.d^{-1}]$	S

Output

$RCR_{bird/mammal}$	risk characterisation ratio for indicator species	[-]	O

Table III-128 Default settings of the model for primary poisoning.

Parameter	**Symbol**	**Unit**	**Value**
Fraction of active substance in product	Fsubst	[-]	-
Daily food intake rate of indicator species	DFI	$[kg_{food}.d^{-1}]$	equation 464-467
Body weight of indicator species	BW	$[kg_{BW}]$	***Table III-120***
Avoidance factor (1= no avoidance, 0 = complete avoidance)	AV	[-]	
bird			1.0
mammal			1.0
Fraction of diet obtained in treated area (value between 0 and 1)	PT	[-]	
bird			0.2
mammal			1.0
Fraction of food type in diet (number between 0 and 1; on or more types)	PD	[-]	
bird			1.0
mammals			
- domestic			0.1
- wild			0.4

Parameters/variables and default values for secondary poisoning.

$$C_{food} = Fsubst \tag{462}$$

$$ETE_{prey\_bird/mammal} = \frac{DFI_{bird/mammal} \cdot C_{food} \cdot AV \cdot PT \cdot PD}{BW_{bird/mammal}} \tag{463}$$

$$IRC_{prey\_bird/mammal} = \sum_{n=1}^{Ndays} ETE_{prey\_bird/mammal} \cdot (1 - Felim_{prey\_bird/mammal})^{n} \tag{464}$$

$$PEC_{oral,predator\_bird/mammal} = \left(IRC_{prey\_bird/mammal,Ndays} + ETE_{prey\_bird/mammal}\right) \cdot F_{prey\_bird/mammal} \tag{465}$$

$$RCR_{predator\_bird/mammal} = \frac{PEC_{oral,predator\_bird/mammal}}{PNEC_{oral,predator}} \tag{466}$$

Input

-	bird species of concern	[-]	P
-	mammalian species of concern	[-]	P
Fsubst	fraction of active substance in product	[-]	S
C_{food}	concentration in food	[$kg_c.kg_{food}^{-1}$]	S/O
$DFI_{bird/mammal}$	daily food intake rate of indicator species	[$kg_{food}.d^{-1}$]	S/O
$BW_{bird/mammal}$	body weight of indicator species	[kg_{BW}]	S/O
AV	avoidance factor	[-]	S/D
PT	fraction of diet obtained in treated area	[-]	S/D
PD	fraction of food type in diet	[-]	S/D
Felim	elimination of the active substance	[-]	S/D
Ndays	number of days the bird/mammal is eating avicide before it is caught by the predator	[-]	S/D
$ETE_{prey\_bird/mammal}$	estimated uptake of a compound by indicator species (prey)	[$kg_c.kg_{BW}^{-1}.d^{-1}$]	O^c
$IRC_{predator\_bird/mammal}$	internal residual concentration in prey after last meal on day = Ndays and before new meal on the next day	[$kg_c.kg_{BW}^{-1}$]	O^c
$PEC_{oral,predator}$	concentration in food, either bird or mammal, of predator	[$kg_c.kg_{food}^{-1}$]	O^c
F_{prey}	fraction of poisoned prey in predator's diet	[-]	D
$PNEC_{oral,predator}$	NOEC for predators	[$kg_c.kg_{food}^{-1}$]	S

Output

$RCR_{predator\_bird/mammal}$	risk characterisation ratio for predator feeding on either (target) birds or mammals	[-]	O

Table III-129 Default settings of the model for secondary poisoning.

Parameter	**Symbol**	**Unit**	**Value**
Fraction of active substance in product	Fsubst	[-]	-
Daily food intake rate of indicator species	DFI	[$kg_{food}.d^{-1}$]	equation 464-467
Body weight of indicator species	BW	[kg_{BW}]	***Table III-120***
Avoidance factor (1= no avoidance, 0 = complete avoidance)	AV	[-]	1.0
Fraction of diet obtained in treated area (value between 0 and 1)	PT	[-]	1.0
bird			0.2
mammal			1.0
Fraction of food type in diet (number between 0 and 1; on or more types)	PD	[-]	
bird			1.0
mammals			
- domestic			0.1
- wild			0.4
Elimination of active substance	Felim	[-]	0.8
Number of days the rodent is eating rodenticide before it is caught by the predator	N_{days}	[-]	
pigeon			5
sparrow			2
Fraction of poisoned prey in predator's diet	F_{prey}		
bird			1.0
mammals			0.5

III.3.6.14 Product type 18: Insecticides

The scenarios and models and calculation formulations used in this version of EUSES 2.1.1 for insecticides have been taken from the following document:

- OECD Series on Emission Scenario Documents.s Number 14 Emission Scenario Document for insecticides for Stables and Manure Storage Systems (2006).This document can be obtained from the ECB Biocides website and from the OECD.
- 4th Draft Emision Scenario Document (ESD) for Insecticides, acaricides and products to control other arthropods (PT 18) for household and professional uses

The following modifications have been made in relation to the scenarios used for insecticides for Stables and Manure Storage Systems:

- Some errors in the original emission scenario documents have been corrected for instance the values for the manure storage area and het housing volume for certain animal categories.
- Also parameters concerning the application regime for both the specific product and manure have been added for some animal categories.
- Some names of parameters have been changed for clarification especially those concerning the timing of biocide and manure application.

The following modifications have been made in relation to the scenarios used for insecticides, acaricides and products to control other arthropods for household and professional uses:

- For calculating the concentration in earthworm (equation 62 in the ESD) an additional factor of 10^4 instead of 10^{-4} is added to convert Tappl expressed in mg/kg into kg/ha.
- All outdoor applications are considered as industrial (professional) use.
- The ESD gives indications for the outdoor spray application to derive local concentrations either in urban area (STP) or in countryside. Although not explicitely mentioned in the ESD, EUSES 2.1.1 also provides the possibly to perform the same exposure assessment for the outdoor spray application in crawling space and outdoor spot application of powders.
- The concentration in earthworm is calculated in accordance to the EU TGD (EC, 2003). Consequently, the ETE for worm-eating birds and mammals are presented in EUSES 2.1.1 in the secondary poisoning screen
- It has also been decided to restrict the secondary poisoning of the outdoor spray application to the calculation of ETE. The calculation of $PNEC_{oral,\ acute/short\ term}$ and RCR has to be done manually

III.3.6.14.1 Insecticides in stables and manure storage systems

The model calculates concentrations in soil and ground water for compounds used as insecticides in stables and manure.

For grassland:

If Tbioc-int > Tgr-int, then

$$Napp - manure = 1 \tag{467}$$

if Tbioc-int < Tgr-int, then

$$Napp - manure = ROUND(Tgr - int/Tbioc - int) \tag{468}$$

if Napp-manure > Napp-bioc$_{max}$, then

$$Napp - manure = Napp - bioc_{\max} \tag{469}$$

For arable land:

$$Tar - int = Tbioc - int \tag{470}$$

and

$$Napp\text{ - }manure = 1 \tag{471}$$

Amount of active ingredient to be used in housing or manure for one application:

[A] $$Qai - prescr_{i1,i2,i3} = 10^{-5} * Qprod - uins_{i1,i2,i3} * Fbioc\% * AREA_{i1}/AREAui_{i1} \tag{472}$$

[B] $$Qai - prescr_{i1,i2,i3} = 10^{-3} * Vprod - uins_{i1,i2,i3} * Fbioc * AREA_{i1}/AREAui_{i1} \tag{473}$$

[C.1] $$Qai - prescri_{i1,i2,i3=2} = 10^{-3} * Qaerosol * VOLUME_{i1}/VOLUMEui_{i1,i2,i3=2} \tag{474}$$

[C.2] $$Qai - prescri_{i1,i2,i3=2} = 10^{-3} * Qaerosol * AREA_{i1}/AREAui_{i1,i2,i3=2} \tag{475}$$

Amount of active ingredient in relevant stream after one application:

[A+B+C] $$Qai_{i1,i2,i3,i4} = F_{i1,i2,i3,i4} * Qai\text{ - }prescr_{i1,i2,i3} \qquad \textbf{(476)}$$

for both application in housings and at manure storage systems, where p is relevant housing category (i1 = 1-18) and q (i1= 19,20) is the relevant storage system:

$$Qai_{tot,i2,i3,i4} = Qai_{p,i2,i3,i4} + Qai_{q,i2,i3,i4} \qquad \textbf{(477)}$$

calculating the amount of active ingredient which goes to manure or slurry for

grassland:

$$Qai - grass_{i1,i2,i3,i4} = Qai_{i1,i2,i3,i4} * Napp - manure_{gr} \qquad \textbf{(478)}$$

arable land:

$$Qai - arab_{i1,i2,i3,i4} = Qai_{i1,i2,i3,i4} * Napp\text{ - }manure_{ar} \qquad \textbf{(479)}$$

calculation of the amount of phosphate and nitrogen in manure produced during the relevant period

$$Qphosph\text{ - }arab_{i1,i4} = N_{i1} * Qphosph_{i1} * Tar - int_{i2} \qquad \textbf{(480)}$$

$$Qphosph\text{ - }grass_{i1,i4} = N_{i1} * Qphosph_{i1} * Tgr - int_{i2} \qquad \textbf{(481)}$$

$$Qnitrog\text{ - }arab_{i1,i4} = N_{i1} * Qnitrog_{i1} * Tar\text{ - }int_{i2} \qquad \textbf{(482)}$$

$$Qnitrog\text{ - }grass_{i1,i4} = N_{i1} * Qnitrog_{i1} * Tgr\text{ - }int_{i2} \qquad \textbf{(483)}$$

Concentration of the active ingredient in soil based on phosphorous or nitrogen immission standards for both grassland and arable land:

$$PIECgrs\text{ - }P2O5_{i1,i2,i3,i4} = \frac{Qai - grass_{i1,i2,i3,i4} * Q_{P2O5,grassland} * 10^{-4}}{Qphosph\text{ - }grass_{i1,i4} * Nlapp - grass * DEPTH_{grassland} * RHOsoil_{wet}}$$

(484)

$$PIECars\text{ - }P2O5_{i1,i2,i3,i4} = \frac{Qai - arab_{i1,i2,i3,i4} * Q_{P2O5,arable\_land} * 10^{-4}}{Qphosph\text{ - }arab_{i1,i4} * Nlapp - arab * DEPTH_{arable\_land} * RHOsoil_{wet}}$$

(485)

$$\mathrm{PIECgrs\text{ - }N}_{\mathrm{i1,i2,i3,i4}} = \frac{\mathrm{Qai - grass}_{\mathrm{i1,i2,i3,i4}} * \mathrm{Q}_{\mathrm{N,grassland}} * 10^{-4}}{\mathrm{Qnitrog\text{ - }grass}_{\mathrm{i1,i4}} * \mathrm{Nlapp - grass} * \mathrm{DEPTH}_{\mathrm{grassland}} * \mathrm{RHOsoil}_{\mathrm{wet}}}$$

(486)

$$\mathrm{PIECars\text{ - }N}_{\mathrm{i1,i2,i3,i4}} = \frac{\mathrm{Qai - arab}_{\mathrm{i1,i2,i3,i4}} * \mathrm{Q}_{\mathrm{N,arable\_land}} * 10^{-4}}{\mathrm{Qnitrog\text{ - }arab}_{\mathrm{i1,i4}} * Nlapp - arab * \mathrm{DEPTH}_{\mathrm{arable\_land}} * \mathrm{RHOsoil}_{\mathrm{wet}}}$$

(487)

Concentration of the active ingredient in ground water and surface water:

Based on phosphate immission standards

$$PIECgrs\text{ - }gw\text{ - }P2O5_{i1,i2,i3,i4} = \frac{PIECgrs\text{ - }P2O5_{i1,i2,i3,i4} * RHOsoil_{wet} * 10^{-3}}{K_{soil-water}} \qquad \mathbf{(488)}$$

$$PIECars\text{ - }gw\text{ - }P2O5_{i1,i2,i3,i4} = \frac{PIECars\text{ - }P2O5_{i1,i2,i3,i4} * RHOsoil_{wet} * 10^{-3}}{K_{soil-water}} \qquad \mathbf{(489)}$$

$$\mathrm{PIECgrs\text{ - }water\text{ - }P2O5_{i1,i2,i3,i4}} = \frac{\mathrm{PIECgrs\text{ - }P2O5_{i1,i2,i3,i4} * RHO_{wet} * 10^{-3}}}{K_{soil-water} * DILUTION_{run-off}} \qquad \mathbf{(490)}$$

$$\mathrm{PIECars\text{ - }water\text{ - }P2O5_{i1,i2,i3,i4}} = \frac{\mathrm{PIECars\text{ - }P2O5_{i1,i2,i3,i4} * RHO_{wet} * 10^{-3}}}{K_{soil-water} * DILUTON_{run-off}} \qquad \mathbf{(491)}$$

Based on nitrogen immision standards

$$PIECgrs\text{ - }gw\text{ - }N_{i1,i2,i3,i4} = \frac{PIECgrs\text{ - }N_{i1,i2,i3,i4} * RHOsoil_{wet} * 10^{-3}}{K_{soil-water}} \qquad \mathbf{(492)}$$

$$PIECars\text{ - }gw\text{ - }N_{i1,i2,i3,i4} = \frac{PIECars\text{ - }N_{i1,i2,i3,i4} * RHOsoil_{wet} * 10^{-3}}{K_{soil-water}} \qquad \mathbf{(493)}$$

$$\mathrm{PIECgrs\text{ - }water\text{ - }N_{i1,i2,i3,i4}} = \frac{\mathrm{PIECgrs\text{ - }N_{i1,i2,i3,i4} * RHO_{wet} * 10^{-3}}}{K_{soil-water} * DILUTION_{run-off}} \qquad \mathbf{(494)}$$

$$\mathrm{PIECars\text{ - }water\text{ - }N_{i1,i2,i3,i4}} = \frac{\mathrm{PIECars\text{ - }N_{i1,i2,i3,i4} * RHO_{wet} * 10^{-3}}}{K_{soil-water} * DILUTION_{run-off}} \qquad \mathbf{(495)}$$

Amount of active ingredient reaching the standard STP for each cleaning event and for the relevant cases of i1 = 8, 11, 12, 16, 17 and 18 when STP = yes

$$\mathrm{Qai\text{ - }STP_{i1,i2,i3,i4}} = \mathrm{F_{i1,i2,i3,i4}} * Qai - prescri_{i1,i2,i3} \qquad \mathbf{(496)}$$

Input

cat-subcat	type of housing or manure storage	[-]	P
bioctype	type of insecticide	[-]	P
appway	type of application n	[-]	P
manstore	type of manure storage	[-]	P
STP	waste water to public sewage treatment plant	[yes/no]	P
AREA$_{i1}$	area of the housing for each category-subcategory	[m^2]	P
VOLUME$_{i1}$	volume of the housing	[m^{-3}]	P
Fbioc%	content of active ingredient in formulation	[%]	S
AREAui$_{i1,i2,i3}$	area to be treated with the amount prescribed	[m^2]	S
Qprod-ui$_{i1,i2,i3}$	amount of product prescribed to be used for specified area	[kg]	S
Fbioc	content of active ingredient in formulation	[kg.m^{-3}]	S
Vprod-ui$_{i1,i2,i3}$	amount of product prescribed to be used for specified area	[m^3]	S
Qaerosol	capacity of one aerosol can	[kg]	S
AREAui$_{i1,i2,i3=2}$	area to treated with one aerosol can	[m^2]	S
VOLUMEui$_{i1,i2,i3=2}$	volume to be treated with one aerosol can	[m^3]	S
F$_{i1,i2,i3,i4}$	fraction of active ingredient released	[-]	D
Napp-bioc$_{max}$	maximum number of repeated treatments prescribed	[-]	S/D
Napp-manure	number of applications during manure storage period	[-]	O
Tbioc-int	insecticide application interval	[d]	S/D
Napp-grass	number of manure applications for grassland	[-]	D
Napp-arab	number of manure applications for arable land	[-]	D
Tgr-int	manure application time interval for grassland	[d]	D
Tar-int	manure application time interval for arable land	[d]	D
N$_{i1}$	number of animals in housing for every relevant category	[-]	D
Qphosph$_{i1}$	amount of phosphate per animal for every category	[kg.d^{-1}]	D
Qnitrog$_{i1}$	amount of nitrogen per animal for every category	[kg.d^{-1}]	D
Q$_{P2O5,grassland}$	phosphate immission standard for one year on grassland	[kg.ha^{-1}]	D
Q$_{P2O5,arable\_land}$	phosphate immission standard for one year on arable land	[kg.ha^{-1}]	D
Q$_{N,grassland}$	nitrogen immission standard for one year on grassland	[kg.ha^{-1}]	D
Q$_{N,arable\_land}$	nitrogen immission standard for one year on arable land	[kg.ha^{-1}]	D
DEPTH$_{grassland}$	mixing depth with soil for grassland	[m]	D
DEPTH$_{arable\_land}$	mixing depth with soil for arable land	[m]	D
RHOsoil$_{wet}$	bulk density of wet soil	[kg.m^{-3}]	D
DILUTIONrun-off	dilution factor for run-off water into surface water	[-]	D
Ksoil-water	soil-water equilibrium partition coefficient	[m$_{water}{}^3$.m$_{soil}{}^{-3}$]	O^c

Output

Qai-prescr$_{i1,i2,i3}$	amount of active ingredient in relevant stream after one application	[kg$_c$]	O^c
Qai-prescr$_{tot,i2,i3}$	total amount of active ingredient in relevant stream after one application in both housing and manure storage system	[kg$_c$]	O^c
Qai-grass$_{i1,i2,i3,i2}$	amount of active ingredient in manure or slurry after the relevant number of biocide applications for the manure application to grass land	[kg$_c$]	O^c
Qai-arab$_{i1,i2,i3,i2}$	amount of active ingredient in manure or slurry after the relevant number of biocide applications for the manure application to arable land	[kg$_c$]	O^c
Qphosph-grass$_{i1,4}$	amount of phosphate produced during the relevant period for every relevant (sub)category of animal housing and application to grassland	[kg]	O^c
Qphosph-arab $_{i1,i4}$	amount of phosphate produced during the relevant period for every relevant (sub)category of animal housing and application to arable land	[kg]	O^c
Qnitrog-grass$_{i1,4}$	amount of nitrogen produced during the relevant period for every relevant (sub)category of animal housing and application to grassland	[kg]	O^c
Qnitrog-arab $_{i1,i4}$	amount of nitrogen produced during the relevant period for every relevant (sub)category of animal housing and application		

	to arable land	[kg]	O^c
PIECgrs-P2O5$_{i1,i2,,i3,i4}$	concentration of active ingredient in soil based on phosphate immission standard for grassland	[kg$_c$.kg^{-1}]	O
PIECarab-P2O5$_{i1,i2,,i3,i4}$	concentration of active ingredient in soil based on phosphate Immission standard for arable land	[kg$_c$.kg^{-1}]	O
PIECgrs-N$_{i1,i2,,i3,i4}$	concentration of active ingredient in soil based on nitrogen immission standard for grassland	[kg$_c$.kg^{-1}]	O
PIECarab-N$_{i1,i2,,i3,i4}$	concentration of active ingredient in soil based on nitrogen immission standard for arable land	[kg$_c$.kg^{-1}]	O
PIECgrs-pw-P$_{i1,i2,,i3,i4}$	concentration of active ingredient in pore water based on phosphate immission standard for grassland	[kg$_c$.kg^{-1}]	O
PIECars-pw-P$_{i1,i2,,i3,i4}$	concentration of active ingredient in pore water based on phosphate immission standard for arable land	[kg$_c$.kg^{-1}]	O
PIECgrs-pw-N$_{i1,i2,,i3,i4}$	concentration of active ingredient in pore water based on nitrogen immission standard for grassland	[kg$_c$.kg^{-1}]	O
PIECars-pw-N$_{i1,i2,,i3,i4}$	concentration of active ingredient in pore water based on nitrogen immission standard for arable land	[kg$_c$.kg^{-1}]	O
PIECgrs-wat-P$_{i1,i2,,i3,i4}$	concentration of active ingredient in water based on phosphate immission standard for grassland	[kg$_c$.kg^{-1}]	O
PIECars-wat-P$_{i1,i2,,i3,i4}$	concentration of active ingredient in water based on phosphate immission standard for arable land	[kg$_c$.kg^{-1}]	O
PIECgrs-wat-N$_{i1,i2,,i3,i4}$	concentration of active ingredient in water based on nitrogen immission standard for grassland	[kg$_c$.kg^{-1}]	O
PIECars-wat-N$_{i1,i2,,i3,i4}$	concentration of active ingredient in water based on nitrogen immission standard for arable land	[kg$_c$.kg^{-1}]	O
Qai-STP$_{i1,i2,i3,i4}$	amount of active ingredient reaching the STP at each cleaning event	[kg$_c$.d^{-1}]	O

Table III-130 Default settings for calculating concentrations in surface water for compounds used as insecticides.

Category-subcategory, i1	**Bioctype, i2**	**Appway, i3**	**Stream, i4**
1) Dairy cows 2) Beef cattle 3) Veal calves 4) Sows in individual pens 5) Sows in groups 6) Fattening pigs 7) Laying hens in battery cages without treatment 8) Laying hens in battery cages with belt drying 9) Laying hens in battery cages with forced drying (deep pit, high-rise) 10) Laying hens in compact battery cages 11) Laying hens in free range with litter floor 12) Broilers in free range with litter floor 13) Laying hens in free range with grating floor (aviary system) 14) Parent broilers in free range with grating floor 15) Parent broilers in rearing with grating floor 16) Turkeys in free range with litter floor 17) Ducks in free range with litter floor 18) Geese in free range with litter floor 19) Wet manure storage (slurry pits) 20) Dry manure storage (manure heaps)	1) Insecticide against adult flies 2) Insecticide against bloodsucking pests 3) Larvicide 4) Insecticide against insects not affecting live stock	1) Spraying 2) Aerosol/fogging 3) Smearing 4) Sprinkling 5) Bait 6) Bait and sprinkling	1) Dry manure 2) Waste water 3) Slurry

Table III-131 Default settings for parameters used in calculating the amount of active ingredient applied and the amount of manure produced: Number of animals, N_{i1} [-], floor $AREA_{i1}$ [m^2], housing volume [m3], amount of phosphate produced, $Qphosph_{i1}$, [$kg.animal^{-1}.day^{-1}$], amount of nitrogen produced, $Qnitrog_{i1}$, [$kg.animal^{-1}.day^{-1}$] and the manure area for manure storage systems $AREA_{i1=19,20}$ [m^2]

Category-subcategory	**Subcategory**	**N_{i1}**	**$Qphosph_{i1}$**	**$Qnitrog_{i1}$**		**$AREA_{i1=19,20}$**		
					Dry storage	**Wet storage (slurry)**		
					Manure heaps	**Tank**		**Lagoon**
						Rectangular	**Circular**	
Cattle								
Dairy		100	0.10466	0.33890	n.r.	1515	1238	4086
Beef		125	0.07123	0.28819	n.r.	495	404	1175
Veal calves		80	0.01422	0.02382	n.r.	319	261	695
Pigs								
Sows	individual	132	0.05566	0.07106	n.r.	369	301	823
	group	132	0.05566	0.07106	n.r.	369	301	823
Fattening pigs		400	0.02033	0.03043	n.r.	369	301	985
Poultry								
Laying hens	Battery-no treatment	21000	0.00111	0.00181	n.r.	350	280	759
	Battery-belt drying	21000	0.00111	0.00181	750	n.r.	n.r.	n.r.
	Battery-deep pit high rise	21000	0.00111	0.00181	750	n.r.	n.r.	n.r.
	Compact	21000	0.00122	0.00202	n.r.	350	280	759
	Free-range litter floor	10000	0.00111	0.00171	360	n.r.	n.r.	n.r.
	Aviary	20000	0.00111	0.00171	n.r.	330	270	731
Broilers	Free-range litter floor	20000	0.00066	0.00156	500	n.r.	n.r.	n.r.
Parent broilers	Free-range grating floor	7000	0.00077	0.00137	n.r.	131	107	267
Parent broilers in rearing	Free-range grating floor	9000	0.00188	0.00298	n.r.	155	127	316
Turkey	Free-range litter floor	10000	0.00230	0.00482	1160	n.r.	n.r.	n.r.
Ducks	Free-range litter floor	10000	0.00164	0.00274	470	n.r.	n.r.	n.r.
Geese	Free-range litter floor	10000	0.00230	0.00482	1160	n.r.	n.r.	n.r.

n.r. not relevant

Table III-132 Defaults for surfaces of manure and spilled feeding, inside the housing specifically for larvicides and the surface area for insecticides in addition to walls, floors and ceiling, for battery systems: $AREA_{i1}$ [m^2], housing volume [m3].

Category-subcategory	**Subcategory**	**N_{i1}**	**$AREA_{i1}$**		**$VOLUME_{i1}$**	**$AREA_{i1}$**		
			floor	**wall and roof**		**Slatted area**	**Other areas**	**Manure area inside**
Cattle								
Dairy		100	1170	1670	9630	360	30	
Beef		125	370	1000	3063	340	40	
Veal calves		80	160	330	590	140	20	
Pigs								
Sows	individual	132	560	910	1960	390	70	
	group	132	710	1160	2480	290	40	
Fattening pigs		400	600	970	2110	400	50	
Poultry								
Laying hens	Battery-no treatment	21000	750	1100	2810	n.r.	1360	1200
	Battery-belt drying	21000	750	1100	2810	n.r.	1360	1200
	Battery-deep pit high rise	21000	750	1100	2810	n.r.	1360	600
	Compact	21000	750	1100	2810	n.r.	1360	300
	Free-range litter floor	10000	1430	2030	5360	950	200	
	Aviary	20000	1270	1822	4780	n.r.	300	1600
Broilers	Free-range litter floor	20000	1110	1600	4170	n.r.	20	
Parent broilers	Free-range grating floor	7000	390	600	1458	260	40	
Parent broilers in rearing	Free-range grating floor	9000	500	750	1880	330	60	
Turkey	Free-range litter floor	10000	3330	4650	12500	n.r	60	
Ducks	Free-range litter floor	10000	2000	2820	7500	n.r.	60	
Geese	Free-range litter floor	10000	2500	3500	9380	n.r.	60	

n.r. not relevant

Table III-133 Default emission factors for spraying for relevant streams for type of animals and housing (sub)category, type of insecticide.

Category-subcat	**Adult flies (1)**			**Bloodsucking pests (2)**			**Larvicides (3)**			**Not affecting livestock (4)**		
	Manure	**Water**	**Slurry**	**Manure**	**Water**	**Slurry**	**Manure**	**Water**	**Slurry**	**Manure**	**Water**	**Slurry**
1			0.5			0.5			0.5			0.5
2			0.5			0.5			0.5			0.5
3			0.5			0.5			0.5			0.5
4			0.5			0.5			0.5			0.5
5			0.5			0.5			0.5			0.5
6			0.5			0.5			0.5			0.5
7			0.5			0.5			0.5			0.5
8		0.2	0.5		0.2	0.5		0.2	0.5		0.2	0.5
9	0.8			0.5			0.8			0.5		
10			0.5			0.5			0.5			0.5
11	0.3	0.2		0.3	0.2		0.3	0.2		0.3	0.2	
12	0.3	0.2		0.3	0.2		0.3	0.2		0.3	0.2	
13			0.5			0.5			0.5			0.5
14			0.5			0.5			0.5			0.5
15			0.5			0.5			0.5			0.5
16	0.3	0.2		0.3	0.2		0.3	0.2		0.3	0.2	
17	0.3	0.2		0.3	0.2		0.3	0.2		0.3	0.2	
18	0.3	0.2		0.3	0.2		0.3	0.2		0.3	0.2	
19a									1.0			
19b									1.0			
19c									1.0			
20a									1.0			
20b							1.0					
20c							1.0					

19a: i1=1-6; 19b: i1=7,10; 19c: i1=13-15; 20a: i1=8; 20b: i1=9; 20c: i1=11,12,16,17,18

Table III-134 Default emission factors for aerosol for relevant streams for type of animals and housing (sub)category, type of insecticide.

Category-subcat	Adult flies (1)			Bloodsucking pests (2)			Larvicides (3)			Not affecting livestock (4)		
	Manure	Water	Slurry	Manure	Water	Slurry	Manure	Water	Slurry	Manure	Water	Slurry
1			0.35			0.35			0.35			0.35
2			0.35			0.35			0.35			0.35
3			0.35			0.35			0.35			0.35
4			0.35			0.35			0.35			0.35
5			0.35			0.35			0.35			0.35
6			0.35			0.35			0.35			0.35
7			0.35			0.35			0.35			0.35
8		0.10	0.35		0.10	0.35		0.10	0.35		0.10	0.35
9	0.35			0.35			0.35			0.35		
10			0.35			0.35			0.35			0.35
11	0.25	0.10		0.25	0.10		0.25	0.10		0.25	0.10	
12	0.25	0.10		0.25	0.10		0.25	0.10		0.25	0.10	
13			0.35			0.35			0.35			0.35
14			0.35			0.35			0.35			0.35
15			0.35			0.35			0.35			0.35
16	0.25	0.10		0.25	0.10		0.25	0.10		0.25	0.10	
17	0.25	0.10		0.25	0.10		0.25	0.10		0.25	0.10	
18	0.25	0.10		0.25	0.10		0.25	0.10		0.25	0.10	
19a									1.0			
19b									1.0			
19c									1.0			
20a									1.0			
20b							1.0					
20c							1.0					

19a: i1=1-6; 19b: i1=7,10; 19c: i1=13-15; 20a: i1=8; 20b: i1=9; 20c: i1=11,12,16,17,18

Table III-135 Default emission factors for smearing for relevant streams for type of animals and housing (sub)category, type of insecticide.

Category-subcat	**Adult flies (1)**			**Bloodsucking pests (2)**			**Larvicides (3)**			**Not affecting livestock (4)**		
	Manure	**Water**	**Slurry**	**Manure**	**Water**	**Slurry**	**Manure**	**Water**	**Slurry**	**Manure**	**Water**	**Slurry**
1			0.35			0.35			0.35			0.35
2			0.35			0.35			0.35			0.35
3			0.35			0.35			0.35			0.35
4			0.35			0.35			0.35			0.35
5			0.35			0.35			0.35			0.35
6			0.35			0.35			0.35			0.35
7			0.35			0.35			0.35			0.35
8		0.10	0.35		0.10	0.35		0.10	0.35		0.10	0.35
9	0.35			0.35			0.35			0.35		
10			0.35			0.35			0.35			0.35
11	0.25	0.10		0.25	0.10		0.25	0.10		0.25	0.10	
12	0.25	0.10		0.25	0.10		0.25	0.10		0.25	0.10	
13			0.35			0.35			0.35			0.35
14			0.35			0.35			0.35			0.35
15			0.35			0.35			0.35			0.35
16	0.25	0.10		0.25	0.10		0.25	0.10		0.25	0.10	
17	0.25	0.10		0.25	0.10		0.25	0.10		0.25	0.10	
18	0.25	0.10		0.25	0.10		0.25	0.10		0.25	0.10	
19a												
19b												
19c												
20a												
20b							1.0					
20c												

19a: i1=1-6; 19b: i1=7,10; 19c: i1=13-15; 20a: i1=8; 20b: i1=9; 20c: i1=11,12,16,17,18

Table III-136 Default emission factors for sprinkling for relevant streams for type of animals and housing (sub)category, type of insecticide.

Category-subcat	**Adult flies (1)**			**Bloodsucking pests (2)**			**Larvicides (3)**			**Not affecting livestock(4)**		
	Manure	**Water**	**Slurry**	**Manure**	**Water**	**Slurry**	**Manure**	**Water**	**Slurry**	**Manure**	**Water**	**Slurry**
1			0.90			0.90						0.90
2			0.90			0.90						0.90
3			0.90			0.90						0.90
4			0.90			0.90						0.90
5			0.90			0.90						0.90
6			0.90			0.90						0.90
7			0.90			0.90			0.90			0.90
8								0.10	0.90			
9	0.90			0.80			0.90			0.80		
10			0.90			0.90			0.90			0.90
11	0.80	0.10		0.80	0.10		0.80	0.10		0.80	0.10	
12	0.80	0.10		0.80	0.10		0.80	0.10		0.80	0.10	
13			0.90			0.90			0.90			0.90
14			0.90			0.90			0.90			0.90
15			0.90			0.90			0.90			0.90
16	0.80	0.10		0.80	0.10		0.80	0.10		0.80	0.10	
17	0.80	0.10		0.80	0.10		0.80	0.10		0.80	0.10	
18	0.80	0.10		0.80	0.10		0.80	0.10		0.80	0.10	
19a									1.0			
19b									1.0			
19c									1.0			
20a									1.0			
20b							1.0					
20c							1.0					

19a: i1=1-6; 19b: i1=7,10; 19c: i1=13-15; 20a: i1=8; 20b: i1=9; 20c: i1=11,12,16,17,18

Table III-137 Default emission factors for bait for relevant streams for type of animals and housing (sub)category, type of insecticide.

Category-subcat	**Adult flies (1)**			**Bloodsucking pests (2)**			**Larvicides (3)**			**Not affecting livestock (4)**		
	Manure	**Water**	**Slurry**	**Manure**	**Water**	**Slurry**	**Manure**	**Water**	**Slurry**	**Manure**	**Water**	**Slurry**
1			0.50			0.50						0.50
2			0.50			0.50						0.50
3			0.50			0.50						0.50
4			0.50			0.50						0.50
5			0.50			0.50						0.50
6			0.50			0.50						0.50
7			0.50			0.50						0.50
8		0.45	0.50		0.45	0.50					0.45	0.50
9	0.50			0.40						0.40		
10			0.50			0.50						0.50
11	0.05	0.45		0.05	0.45					0.05	0.45	
12	0.05	0.45		0.05	0.45					0.05	0.45	
13			0.50			0.50						0.50
14			0.50			0.50						0.50
15			0.50			0.50						0.50
16	0.05	0.45		0.05	0.45					0.05	0.45	
17	0.05	0.45		0.05	0.45					0.05	0.45	
18	0.05	0.45		0.05	0.45					0.05	0.45	
19a												
19b												
19c												
20a												
20b												
20c												

19a: i1=1-6; 19b: i1=7,10; 19c: i1=13-15; 20a: i1=8; 20b: i1=9; 20c: i1=11,12,16,17,18

Table III-138 Default emission factors for bait and sprinkling for relevant streams for type of animals and housing (sub)category, type of insecticide.

Category-subcat	**Adult flies (1)**			**Bloodsucking pests (2)**			**Larvicides (3)**			**Not affecting livestock (4)**		
	Manure	**Water**	**Slurry**	**Manure**	**Water**	**Slurry**	**Manure**	**Water**	**Slurry**	**Manure**	**Water**	**Slurry**
1			0.75			0.75						0.75
2			0.75			0.75						0.75
3			0.75			0.75						0.75
4			0.75			0.75						0.75
5			0.75			0.75						0.75
6			0.75			0.75						0.75
7			0.75			0.75						0.75
8		0.35	0.75		0.35	0.75					0.35	0.75
9	0.80			0.75						0.75		
10			0.75			0.75						0.75
11	0.40	0.35		0.40	0.35					0.40	0.35	
12	0.40	0.35		0.40	0.35					0.40	0.35	
13			0.75			0.75						0.75
14			0.75			0.75						0.75
15			0.75			0.75						0.75
16	0.40	0.35		0.40	0.35					0.40	0.35	
17	0.40	0.35		0.40	0.35					0.40	0.35	
18	0.40	0.35		0.40	0.35					0.40	0.35	
19a												
19b												
19c												
20a												
20b												
20c												

19a: i1=1-6; 19b: i1=7,10; 19c: i1=13-15; 20a: i1=8; 20b: i1=9; 20c: i1=11,12,16,17,18

Table III-139 Default settings for the application interval Tbioc-int and the maximum number of applications Napp-bioc$_{max}$.

Index i2	Index i1	Napp-bioc$_{max}$	Tbioc-int
1	1-18	6	28
2	7-10	4	91
2	11,13	4	91
2	12, 17, 18	7	52
2	14	4	91
2	15	4	91
2	16	3	122
3	1-20	6	28
4	7-11,13,14	1	365
4	12, 17, 18	7	52
4	15, 16	3	122

Table III-140 Default values for the manure storage time interval Tar/gr-int [d] by target field.

Target field	Tar/gr-int
Arable land	212
Grass land	53

Table III-141 Maximum immission standards [kg.ha^{-1}.yr^{-1}] on arable and grassland for nitrogen and phosphate Default settings for the application interval Tbioc-int and the maximum number of applications Napp-bioc$_{max}$.

Country	**Arable**		**Grass**	
	$Q_{N,arable\_land}$	**$Q_{P2O5,arable\_land}$**	**$Q_{N,grassland}$**	**$Q_{P2O5,grassland}$**
Belgium	120		280	
Denmark	140		230	
Finland	130		250	
France	170		170	
Germany	170		210	
Italy	170		170	
Ireland	170		210	
The Netherlands	170	85	170$^{3)}$	110
Portugal	250		250	
Spain	170		210	
Sweden	170		170	
United Kingdom	210		250	

Table III-142 Default values for the number of land application per year, Nlapp-grass and Nlapp-arab [yr^{-1}] and the mixing depth for soil DEPTH [m].

Target field	**Nlapp**	**DEPTH**
Arable land	1	0.20
Grass land	4	0.05

III.3.6.14.2 Insecticides, acaricides and products to control other arthropods for household and professional uses

Indoor spray application (18.2.1)

Mixing loading step

Parameters/variables and default values for mixing loading step of indoor spray application.

$$F_{prep,applicator} + F_{prep,air} + F_{prep,floor} + F_{prep,treated} = 1 \qquad \textbf{(497)}$$

$$Q_{prod,prep} = \frac{((Vol / AREA_{treated} \cdot Q_{ai}) / F_{ai})}{N_{prep}} \qquad \textbf{(498)}$$

$$E_{prep,air} = \frac{(Q_{prod,prep} \cdot F_{ai} \cdot N_{prep} \cdot F_{prep,air})}{1000} \qquad \textbf{(499)}$$

$$E_{prep,applicator} = \frac{(Q_{prod,prep} \cdot F_{ai} \cdot N_{prep} \cdot F_{prep,applicator})}{1000} \quad \text{(STP)} \quad \textbf{(500)}$$

$$E_{prep,floor} = \frac{(Q_{prod,prep} \cdot F_{ai} \cdot N_{prep} \cdot F_{prep,floor})}{1000} \quad \text{(STP)} \quad \textbf{(501)}$$

Input			
F_{ai}	Fraction of active ingredient in product	[-]	S
Q_{ai}	Treatment rate	[g.m2 or g.m3]	S
$F_{prep,air,}$	Fraction emitted to the air during the mixing/ loading step for the application by spraying	[-]	D
$F_{prep,floor}$	Fraction emitted to the floor during the mixing/ loading step for the application by spraying	[-]	P
$F_{prep,applicator}$	Fraction emitted to the applicator during the mixing/ loading step for the application by spraying	[-]	P
N_{prep}	Number of preparations per day	[-]	P
$VOL/AREA_{treated}$	Treated volume / area	[m2 or m3]	D
Output			
$Q_{prod,prep}$	Quantity of commercial product used for the preparation per building	[g]	O
$E_{prep,air}$	Emission to air	[kg.d-1]	O
$E_{prep, applicator}$	Emission to applicator	[kg.d-1]	O
$E_{prep, floor}$	Emission to the floor	[kg.d-1]	O

Table III-143 Default values for the mixing step of the indoor spray application.

Parameter	**Value**
N_{prep}	House (1, professional and non-professional), larger building (3, professional)
$F_{prep,air}$	0
$F_{prep,applicator}$	Liquid (0.0012), powder (0), granules (0)
$VOLUME_{treated}$	58
$AREA_{treated}$	General surface treatment (22), targeted spot (2), larger building treatment (3280)

Table III-144 *:* Emission factors to floor expressed as ml of commercial product per operation for containers with unspecific design (PSD 1992).

Container volume	Losses to the hands	Losses to the floor		$F_{prep,\ floor,i}$	
		Professional	General public user	Professional	General public user
1 liter	0.01 ml	0.1 ml	1 ml	10^{-4}	10^{-3}
5 litres	0.2 ml	2 ml	20 ml	4.10^{-4}	4.10^{-3}
10 litres	0.5 ml	5 ml	50 ml	5.10^{-4}	5.10^{-3}
20 litres	0.5 ml	5 ml	50 ml	$2.5.10^{-4}$	$2.5.10^{-3}$

Table III-145 Emission factors to floor expressed as ml of commercial product per operation for wide-necked container (PSD 1992)

Container volume	Losses to the hands	Losses to the floor		$F_{prep,\ floor,i}$	
		Professional	General public user	Professional	General public user
1 liter D* = all	0.01 ml	0.1 ml	1 ml	10^{-4}	10^{-3}
2 litres D = all	0.01 ml	0.1 ml	1 ml	5.10^{-5}	5.10^{-4}
5 litres D = 45/63 mm	0.01 ml	0.1 ml	1 ml	2.10^{-5}	2.10^{-4}
10 litres D=45 mm	0.1 ml	1 ml	10 ml	10^{-4}	10^{-3}
10 litres D=63 mm	0.05 ml	0.5 ml	5 ml	5.10^{-5}	5.10^{-4}

*D = neck diameter

Application step

Parameters/variables and default values for application step of indoor spray application.

$$F_{appl,applicator} + F_{appl,air} + F_{appl,floor} + F_{appl,treated} = 1 \qquad \textbf{(502)}$$

$$Q_{prod,appli} = \frac{((Vol / AREA_{treated} \cdot Q_{ai}) / F_{ai})}{N_{appl}} \qquad \textbf{(503)}$$

Air space treatment

$$E_{appl,air} = \frac{(N_{appl} \cdot F_{appl,air} \cdot Q_{prod,appl} \cdot F_{ai} \cdot VOL_{treated})}{1000} \qquad \textbf{(504)}$$

$$E_{appl,applicator} = \frac{(N_{appl} \cdot F_{applicator} \cdot Q_{prod,appl} \cdot F_{ai} \cdot VOL_{treated})}{1000} \qquad \text{(STP)} \quad \textbf{(505)}$$

$$E_{appl,floor} = \frac{(N_{appl} \cdot F_{appl,floor} \cdot Q_{prod,appl} \cdot F_{ai} \cdot VOL_{treated})}{1000} \qquad \text{(STP)} \quad \mathbf{(506)}$$

$$E_{appl,treated} = \frac{(N_{appl} \cdot F_{appl,treated} \cdot Q_{prod,appl} \cdot F_{ai} \cdot VOL_{treated})}{1000} \qquad \text{(STP)} \quad \mathbf{(507)}$$

Table III-146 Default values for the application step of the indoor spray application, air space treatment

parameter	**value**
$N_{appl,building}$	Non-professional (4), professional (-)
$VOLUME_{treated}$	General air space application (58), larger building (not specified)
$F_{appl,air}$	0.02
$F_{appl,floor}$	0.96
$F_{appl,treated}$	0
$F_{appl,applicator}$	0.02

Treatment of a surface

$$E_{appl,air} = \frac{(N_{appl} \cdot F_{appl,air} \cdot Q_{prod,appl} \cdot F_{ai} \cdot AREA_{treated})}{1000} \quad \mathbf{(508)}$$

$$E_{appl,applicator} = \frac{(N_{appl} \cdot F_{applicator} \cdot Q_{prod,appl} \cdot F_{ai} \cdot AREA_{treated})}{1000} \quad \mathbf{(509)}$$

$$E_{appl,floor} = \frac{(N_{appl} \cdot F_{appl,floor} \cdot Q_{prod,appl} \cdot F_{ai} \cdot AREA_{treated})}{1000} \quad \mathbf{(510)}$$

$$E_{appl,treated} = \frac{(N_{appl} \cdot F_{appl,treated} \cdot Q_{prod,appl} \cdot F_{ai} \cdot AREA_{treated})}{1000} \quad \mathbf{(511)}$$

Table III-147 Default values for the application step of the indoor spray application, treatment of a surface

parameter	**value**
$N_{appl,building}$	Non-professional (1), professional (-)
$AREA_{treated}$	target spot application (2), general spray application / household (22), larger building (3280)
$F_{appl,air}$	0.02
$F_{appl,floor}$	0.11
$F_{appl,treated}$	0.85
$F_{appl,applicator}$	0.02

Input

F_{ai}	Fraction of active ingredient in product	[-]	S
Q_{ai}	Treatment rate	[g.m2 or g.m3]	S

$F_{appl,air,}$	Fraction emitted to the air during application	[-]	P
$F_{appl,floor}$	Fraction emitted to the floor during application	[-]	P
$F_{appl,applicator}$	Fraction emitted to the applicator during application	[-]	P
$F_{appl,treated}$	Fraction emitted to the treated surfaces during application	[-]	P
N_{appl}	Number of applications per day per building	[d-1]	P
$VOL/AREA_{treated}$	Treated volume / area	[m2 or m3]	D
Output			
$Q_{prod,appl}$	uantity of commercial product used for the preparation per building	[g]	O
$E_{appl,air}$	Emission to air	[kg.d-1]	O
$E_{appl, applicator}$	Emission to applicator	[kg.d-1]	O
$E_{appl, floor}$	Emission to the floor	[kg.d-1]	O
$E_{appl,treated}$	Emission to treated surface/volume	[kg.d-1]	O

Cleaning step

Parameters/variables and default values for cleaning step of indoor spray application.

Release to air

$E_{cleaning,air} = 0$ (outdoor air)

No release to waste water

$$E_{applicator,w} = (E_{prep,applicator} + E_{application,applicator}) \cdot F_{applicator,w} \qquad \textbf{(512)}$$

$$E_{treated,w} = (E_{prep,floor} + E_{application,floor} + E_{application,treated}) \cdot F_{w} \cdot F_{CE} \qquad \textbf{(513)}$$

If 100% of the coveralls are disposable, then $F_{applicator,w} = 1$ and $F_{applicator,ww} = 0$.
If 100% of the surfaces are cleaned by vacuum/broom, then $F_{w} = 1$ and $F_{ww} = 0$.

Input			
$E_{prep,applicator}$	Emission to applicator during preparation step	[kd.d-1]	O
$E_{application,applicator}$	Emission to applicator during the application step	[kg.d-1]	O
$F_{applicator,w}$	Fraction emitted to solid waste from applicator	[-]	P
$E_{prep,floor}$	Emission to the floor during preparation	[kg.d-1]	O
$E_{application,floor}$	Emission to the floor during application	[kg.d-1]	O
$E_{application,treated}$	Emission to treated surfaces during the application step	[kg.d-1]	O
F_{w}	Fraction emitted to solid waste	[-]	D
F_{CE}	Cleaning efficiency	[-]	D
Output			
$E_{applicator,w}$	Emission from applicator to solid waste during cleaning	[kg.d-1]	
$E_{treated,w}$	Emission from floor/treated surfaces to solid waste	[kg.d-1]	

No release to municipal wastes

$$E_{applicator,ww} = (E_{prep,applicator} + E_{application,applicator}) \cdot F_{applicator,ww} \qquad \textbf{(514)}$$

$$E_{treated,ww} = (E_{prep,floor} + E_{application,floor} + E_{application,treated}) \cdot F_{ww} \cdot F_{CE} \qquad \textbf{(515)}$$

If 100% of the coveralls are washable, then $F_{applicator,w} = 0$ and $F_{applicator,ww} = 1$.
If 100% of the surfaces are cleaned by water, then $F_w = 0$ and $F_{ww} = 1$.

Input

$E_{prep,applicator}$	Emission to applicator during preparation step	[kd.d-1]	O
$E_{application,applicator}$	Emission to applicator during the application step	[kg.d-1]	O
$F_{applicator,ww}$	Fraction emitted to waste water from applicator	[-]	P
$E_{prep,floor}$	Emission to the floor during preparation	[kg.d-1]	O
$E_{application,floor}$	Emission to the floor during application	[kg.d-1]	O
$E_{application,treated}$	Emission to treated surfaces during the application step	[kg.d-1]	O
F_{ww}	Fraction emitted to waste water	[-]	D
F_{CE}	Cleaning efficiency	[-]	D

Output

$E_{applicator,ww}$	Emission from applicator to waste water	[kg.d-1]
$E_{treated,ww}$	Emission from floor/treated surfaces to waste water	[kg.d-1]

Table III-148 Cleaning efficiency for different products used (CEFIC Insecticides Working Group)

Formulation / Use	Maximum % exposed to cleaning (either wet or dry methods)	Cleaning efficiency
Solid Baits (in bait stations)	0	0
Gel – Bait station	0	0
Gels – Crack and crevice	3	0.03
Gels - Surface	25	0.25
Dust / powders Voids / cavities	0	0
Dust/powders – Surface	50	0.5
Spray – Crack and crevice	25	0.25
Spray - Surface	50	0.5
RTU Aerosols – Space Spray/diffuser	100	1
RTU Aerosol – Crack and crevice (including foams)	3	0.03
RTU Aerosols – Surface	20	0.2

Total release

$$E_{total} = ((E_{applicator,w} + E_{treated,w})_{house} \cdot N_{houses} + (E_{applicator,w} + E_{treated,w})_{building} \cdot N_{building}) \cdot F_{simultaneity}$$

(516)

Input

$E_{applicator,ww}$	Emission from applicator to waste water	[kg.d-1]
$E_{treated,ww}$	Emission from floor/treated surfaces to waste water	[kg.d-1]
Nhouses	Number of houses by STP	[-]
Nbuilding	Number of buildings by STP	[-]
$F_{simultaneity}$	Simultaneity factor	[-]

Output

E_{total}	Total Emission to waste water	[kg.d-1]

Table III-149 Default values for the application step of the indoor spray application

parameter	**value**

N_{houses}	4000
$N_{building}$	1000
$F_{simultaneity}$	0.055

Indoor gel application (18.2.2)

Mixing / loading step

No emission during mixing / loading.

Application step

Parameters/variables and default values for application step of indoor gel application.

$$E_{appl,air} = \frac{(Q_{prod,point} \cdot N_{point} \cdot F_{ai} \cdot AREA_{treated} \cdot F_{appl,air} \cdot N_{appl,building})}{1000} \quad \textbf{(517)}$$

$$E_{appl,applicator} = \frac{(Q_{prod,point} \cdot N_{point} \cdot F_{ai} \cdot AREA_{treated} \cdot F_{appl,applicator} \cdot N_{appl,building})}{1000} \quad \text{(STP)} \quad \textbf{(518)}$$

$$E_{appl,treated} = \frac{(Q_{prod,point} \cdot N_{point} \cdot F_{ai} \cdot AREA_{treated} \cdot F_{appl,treated} \cdot N_{appl,building})}{1000} \quad \text{(STP)} \quad \textbf{(519)}$$

Input

F_{ai}	Fraction of active ingredient in product	[-]	S
N_{point}	Number of gel points per square meter	[point.m-2]	P
N_{appl}	Number of applications per day per building	[d-1]	P
$F_{appl,air,}$	Fraction emitted to the air during application	[-]	P
$F_{appl,applicator}$	Fraction emitted to the applicator during application	[-]	P
$F_{appl,treated}$	Fraction emitted to the treated surfaces during application	[-]	P
$AREA_{treated}$	Area treated with the product	[m2]	D
$Q_{prod,point}$	Quantity of commercial product applied per point of gel	[g.point-1]	S

Output

$E_{appl,air}$	Emission to air	[kg.d-1]	O
$E_{appl, applicator}$	Emission to applicator	[kg.d-1]	O
$E_{appl,treated}$	Emission to treated surface/volume	[kg.d-1]	O

Table III-150 Default values for the application step of the indoor gel application

parameter	**value**
$N_{appl,building}$	Household (6), larger building (-)
N_{point}	Preventive treatment or low infestation level (1), curative treatment or high infestation level (3)
$AREA_{treated}$	Household (22), larger building (3280)
$F_{appl,air}$	0
$F_{appl,applicator}$	0

$F_{appl,treated}$	1

Cleaning step

The calculation method is *mutatis mutandis* the same as used for spray application.

Total release

The calculation method is *mutatis mutandis* the same as used for spray application.

Indoor application of powders by dusting (18.2.3)

Mixing / loading step

Parameters/variables and default values for mixing/loading step of indoor application of powders by dusting.

$$E_{prep,air} = \frac{(Q_{prod,prep} \cdot F_{ai} \cdot N_{prep,building} \cdot F_{prep,air})}{1000} \qquad \textbf{(520)}$$

$$E_{prep,floor} = \frac{(Q_{prod,prep} \cdot F_{ai} \cdot N_{prep,building} \cdot F_{prep,floor})}{1000} \qquad \text{(STP)} \quad \textbf{(521)}$$

$$E_{prep,applicator} = \frac{(Q_{prod,prep} \cdot F_{ai} \cdot N_{prep,building} \cdot F_{prep,applicator})}{1000} \qquad \text{(STP)} \quad \textbf{(522)}$$

Input			
F_{ai}	Fraction of active ingredient in product	[-]	S
N_{prep}	Number of preparations per dayper building	[d-1]	P
Output			
$Q_{prod,prep}$	Quantity of commercial product used for the preparation per building	[g]	S
$E_{prep,air}$	Emission to air	[kg.d-1]	O
$E_{prep, applicator}$	Emission to applicator	[kg.d-1]	O
$E_{prep, floor}$	Emission to the floor	[kg.d-1]	O

Table III-151 Default values for the mixing/loading step of the indoor application of powders by dusting

parameter	value
$N_{prep,building}$	House (1), larger building (3)
$F_{prep,air}$	0
$F_{prep,applicator}$	0
$F_{prep,floor}$	0.01

Application step

Parameters/variables and default values for application step of indoor application of powders by dusting.

$$E_{application,air} = N_{appl,building} \cdot F_{application,air} \cdot Q_{prod} \cdot F_{ai} \cdot AREA_{treated} \qquad \textbf{(523)}$$

$$E_{application,treated} = N_{appl,building} \cdot F_{application,treated} \cdot Q_{prod} \cdot F_{ai} \cdot AREA_{treated} \qquad \text{(STP)} \quad \textbf{(524)}$$

$$E_{application,floor} = N_{appl,building} \cdot F_{application,floor} \cdot Q_{prod} \cdot F_{ai} \cdot AREA_{treated} \qquad \text{(STP)} \quad \textbf{(525)}$$

$$E_{application,applicator} = N_{appl,building} \cdot F_{application,applicator} \cdot Q_{prod} \cdot F_{ai} \cdot AREA_{treated} \qquad \text{(STP)} \quad \textbf{(526)}$$

Input			
$N_{appl,building}$	Number of applications per day per building	[d-1]	D
$F_{application,air}$	Fraction emitted to air during application	[-]	D
$F_{applicationtreated}$	Fraction emitted to treated area during application	[-]	D
$F_{application,floor}$	Fraction emitted to floor during application	[-]	D
$F_{application,applicator}$	Fraction emitted to applicator during application	[-]	D
Q_{prod}	Quantity of product applied	[kg.m-2]	S
F_{AI}	Fraction of active substance in commercial product	[-]	S
$AREA_{treated}$	Area treated with the product	[m2]	P
Output			
$E_{application,air}$	Emission to air during application	[kg.d-1]	O
$E_{application,treated}$	Emission to treated area during application	[kg.d-1]	O
$E_{application,floor}$	Emission to floor during application	[kg.d-1]	O
$E_{application,applicator}$	Emission to applicator during application	[kg.d-1]	O

Table III-152 Default values for the application step of the indoor spray application indoor application of powders by dusting

Parameter	**value**
$AREA_{treated}$	Surface dusting crack and crevice (2), surface dusting broadcast (22), larger building (3280)
$N_{appl,building}$	1
$F_{application,air}$	0.02
$F_{application,treated}$	0.8
$F_{application,Floor}$	0.18
$F_{application,applicator}$	0

Cleaning step

The calculation method is *mutatis mutandis* the same as used for spray application.

Total release

The calculation method is *mutatis mutandis* the same as used for spray application.

Indoor injection (18.2.4)

Mixing/loading step

Parameters/variables and default values for mixing/loading step of indoor injection.

$$E_{prep,air} = \frac{(Q_{prod,prep} \cdot F_{ai} \cdot N_{prep,building} \cdot F_{prep,air})}{1000} \qquad \textbf{(527)}$$

$$E_{prep,floor} = \frac{(Q_{prod,prep} \cdot F_{ai} \cdot N_{prep,building} \cdot F_{prep,floor})}{1000} \qquad \text{(STP)} \quad \textbf{(528)}$$

$$E_{prep,applicator} = \frac{(Q_{prod,prep} \cdot F_{ai} \cdot N_{prep,building} \cdot F_{prep,applicator})}{1000} \qquad \text{(STP)} \quad \textbf{(529)}$$

Input

$Q_{prod,prep}$	Quantity of product used for preparation per building	[g]	S
F_{AI}	Fraction of active substance in the commercial product	[-]	S
$N_{prep,building}$	Number of preparations per day	[-]	D
$F_{prep,air}$	Fraction emitted to air	[-]	D
$F_{prep,applicator}$	Fraction emitted to the applicator	[-]	D
$F_{prep,floor}$	Fraction emitted to the floor	[-]	D

Output

$E_{prep,air}$	Emission to air during the preparation step	[kg.d-1]	O
$E_{prep,applicator}$	Emission to applicator during preparation step	[kg.d-1]	O
$E_{prep,floor}$	Emission to the floor during the preparation step	[kg.d-1]	O

Table III-153 Default values for the mixing/loading step of the indoor injection application

parameter	**value**
$N_{prep,building}$	House (1), larger building (1)
$F_{prep,air}$	0
$F_{prep,applicator}$	See table III-143
$F_{prep,floor}$	See table III-144 and III-145

Application step

Parameters/variables and default values for application step of indoor injection.

$$E_{application,air} = Q_{prod} \cdot N_{drilling} \cdot Wall_{length} \cdot N_{appl,building} \cdot F_{ai} \cdot F_{application,air} \qquad \textbf{(530)}$$

$$E_{application,applicator} = Q_{prod} \cdot N_{drilling} \cdot Wall_{length} \cdot N_{appl,building} \cdot F_{ai} \cdot F_{application,applicator} \qquad \text{(STP)}\textbf{(531)}$$

$$E_{application,floor} = Q_{prod} \cdot N_{drilling} \cdot Wall_{length} \cdot N_{appl,building} \cdot F_{ai} \cdot F_{application,floor} \qquad \text{(STP)} \quad \textbf{(532)}$$

$$E_{application,treated} = Q_{prod} \cdot N_{drilling} \cdot Wall_{length} \cdot N_{appl,building} \cdot F_{ai} \cdot F_{application,treated} \qquad \text{(STP)} \quad \textbf{(533)}$$

Input

$Q_{prod,injecteddrilling}$	Quantity of product used per drilling	[g.drilling-1]	S
F_{AI}	raction of active substance in the commercial product	[-]	S
$N_{appl,building}$	Number of preparations per day	[d-1]	D
$N_{drilling}$	Number of drillings per linear meter	[drilling.m-1]	D
$Wall_{length}$	Length of the perimeter wall of the building	[m]	D
$F_{application,air}$	Fraction emitted to the air during injection	[-]	D
$F_{application,applicator}$	Fraction emitted to applicator during injection	[-]	D
$F_{application,floor}$	Fraction emitted to the floor during injection	[-]	D
$F_{application,treated}$	Fraction emitted to treated material during injection	[-]	D

Output

$E_{application,air}$	Emission to air during application	[kg.d-1]	O

$E_{application,treated}$	Emission to treated area during application	[kg.d-1]	O
$E_{application,floor}$	Emission to floor during application	[kg.d-1]	O
$E_{application,applicator}$	Emission to applicator during application	[kg.d-1]	O

Table III-154 Default values for the application step of the indoor injection application

parameter	**value**
$N_{appl,building}$	House (1), larger building (1)
$Wall_{length}$	House (50), larger building (250)
$F_{application,air}$	0
$F_{application,applicator}$	0.001
$F_{application,floor}$	0.05
$F_{application,treated}$	0.949

Cleaning step

The calculation method is *mutatis mutandis* the same as used for spray application.

Total release

The calculation method is *mutatis mutandis* the same as used for spray application.

Indoor applications of Fumigant/gas (18.2.5)

Mixing/loading step

For the fumigants and gases, the products are always in a ready to use form.

Application step

Parameters/variables and default values for application step of indoor application of fumigant/gas.

$$F_{application,air} + F_{application,applicator} + F_{ret} = 1 \qquad \textbf{(534)}$$

$$F_{application,air} = 1 - F_{ret} \qquad \textbf{(535)}$$

$$E_{local,air} = \frac{(Q_{prod} \cdot (1 - F_{ret}) \cdot (1 - F_{disin}))}{T_{emission}} \qquad \textbf{(536)}$$

$$E_{local,air} = 0.979 \cdot Q_{prod} \qquad \textbf{(537)}$$

Input

Q_{prod}	Amount of product used	[kg]	S
F_{ret}	Fraction of retention in goods	[-]	D
F_{disin}	Fraction of disintegration	[-]	D

$F_{application,applicator}$	Fraction of emission to applicator	[-]	D
$F_{application,air}$	Fraction of emission to air	[-]	D
$T_{emission}$	Number of emission days for treatment	[d]	D
Output			
$E_{local,air}$	Local emission to air during episode	[kg.d-1]	O

Table III-155 Default values for the application step of the indoor application of fumigant/gas

parameter	**value**
F_{ret}	Fumigant (0.02), gas (0.02)
F_{disin}	Fumigant (0.001), gas (0.001)
$F_{application,applicator}$	0
$T_{emission}$	1

Indoor applications of Diffusers (18.2.6)

Mixing/loading step

The products are always sold under a ready to use form. Therefore, no emission is calculated for the preparation step of diffusers.

Application step

Parameters/variables and default values for application step of indoor application of diffusers.

$$E_{application,air} = \frac{(Q_{prod} \cdot F_{ai} \cdot (T_{day} / T_{\max}) \cdot F_{application,air})}{1000} \quad \textbf{(538)}$$

$$E_{application,floor} = \frac{(Q_{prod} \cdot F_{ai} \cdot (T_{day} / T_{\max}) \cdot F_{application,floor})}{1000} \quad \text{(STP)} \quad \textbf{(539)}$$

Input

Q_{prod}	Quantity of product contained in the device	[g]	S
T_{Max}	Maximal duration of use of the diffuser	[h]	S
F_{AI}	Fraction of the active substance in the product	[-]	S
T_{Day}	Duration of use per day	[h.d-1]	D
$F_{application,air}$	Fraction emitted to the air during use	[-]	D
$F_{application,floor}$	Fraction emitted to the floor during use	[-]	D
Output			
$E_{application,air}$	Emission to air during the use of diffuser	[kg.d-1]	O
$E_{application,floor}$	Emission to floor during the use of diffuser	[kg.d-1]	O

Table III-156 Default values for the application step of the indoor application of diffusers

parameter	**value**
T_{Day}	Electrical (8), passive (24)
$F_{application,air}$	0.9
$F_{application,floor}$	0.1

Cleaning step

The calculation method is *mutatis mutandis* the same as used for spray application.

Total release

The calculation method is *mutatis mutandis* the same as used for spray application.

Outdoor applications

Outdoor spray applications - flying insects (18.3.1)

Mixing / loading step (applicable to all scenarios)

Parameters/variables and default values for mixing/loading step of outdoor spray application of flying insects..

$$E_{prep,soil} = \frac{(Q_{prod,prep} \cdot F_{ai} \cdot N_{prep} \cdot F_{prep,soil})}{1000} \qquad \textbf{(540)}$$

$$C_{prep,soil} = \frac{E_{prep,soil}}{V_{prep,soil} \cdot RHO_{soil}} \qquad \textbf{(541)}$$

Emission rural: soil; urban: STP

Input			
$Q_{prod,prep}$	Quantity of product used for one preparation event	[g]	S
F_{AI}	Fraction of active substance in the commercial product	[-]	S
N_{prep}	Number of preparations per day	[d-1]	D/S
$F_{prep,soil}$	Fraction emitted to soil during preparation step	[-]	P
$V_{prep,soil}$	Soil volume for the mixing/loading step	[m3]	D
RHO_{soil}	Bulk density of wet soil	[kg_{ww}.m-3]	D
Output			
$E_{prep,soil}$	Emission to soil during the preparation step	[kg.d-1]	O
$C_{prep,soil}$	Concentration of active substance in soil during mixing	[kg.kg_{ww}-1]	O

Table III-157 Default values for the mixing/loading step of the outdoor spray applications flying insects

parameter	**value**
N_{prep}	Houses (1), larger buildings (3)
$F_{prep,soil}$	See table III-144 abd III-145
$V_{prep,soil}$	0.40
RHO_{soil}	1700

Application step

Parameters/variables and default values for application step of outdoor spray application of flying insects..

$$E_{sprayingwall,soil} = Q_{prod} \cdot F_{ai} \cdot AREA_{wall} \cdot F_{spray,wall} \qquad \textbf{(542)}$$

$$C_{sprayingwall,soil} = \frac{E_{sprayingwall,soil}}{V_{spray,soil} \cdot RHO_{soil}} \qquad \textbf{(543)}$$

Emission rural: soil; urban: STP

Input			
Q_{prod}	Quantity of product applied	[kg.m-2]	S
F_{AI}	Fraction of active substance in the commercial product	[-]	S
$AREA_{wall}$	Area of exterior wall treated per day	[m2.d-1]	P
$F_{spray,wall}$	Fraction emitted to soil during outdoor wall spray appl.	[-]	D
$V_{spray,soil}$	Soil volume around building	[m3]	P
RHO_{soil}	Bulk density of wet soil	[kg_{ww}.m-3]	D
Output			
$E_{sprayingwall,soil}$	Local emission from outdoor spray due to deposition	[kg.d-1]	O
$C_{sprayingwall,soil}$	Local concentration of active ingredient in soil	[kg.kg_{ww}-1]	O

Wash-off of the treated surfaces by rainfall

$$E_{spray,wallwash-off,soil} = Q_{prod} \cdot F_{ai} \cdot AREA_{wall} \cdot F_{spray,wash-off} \qquad \textbf{(544)}$$

Emission rural: soil; urban: STP

Urban areas

$$E_{spray,flying} = E_{sprayingwall,soil} + E_{spray,wall,wash-off,soil} \qquad \textbf{(545)}$$

Emission to STP

Rural areas

$$C_{sprayingwall,soil} = \frac{E_{sprayingwall,soil}}{V_{spray,soil} \cdot RHO_{soil}} \qquad \textbf{(546)}$$

$$C_{spray,wall,wash-off,soil} = \frac{(E_{spray,wall} + E_{spray,wall,wash-off,soil})}{V_{spray,soil} \cdot RHO_{soil}} \qquad \textbf{(547)}$$

$$C_{spray,flying,total} = \frac{(E_{spray,wall} + E_{spray,wall,wash-off,soil})}{V_{spray,soil} \cdot RHO_{soil}} \qquad \textbf{(548)}$$

Input

Q_{prod}	Quantity of product applied	[kg.m-2]	S
F_{AI}	Fraction of active substance in the commercial product	[-]	S
$AREA_{wall}$	Area of exterior wall treated per day	[m2.d-1]	P
$F_{spray,wash-off}$	Fraction emitted to soil due to wash-off by rainfall	[-]	D
$V_{spray,soil}$	Soil volume around building	[m3]	P
RHO_{soil}	Bulk density of wet soil	[kg_{ww}.m-3]	D
Output			
$E_{spray,wall,wash-off,soil}$	Local emission from spray due to wash-off	[kg.d-1]	O
$E_{spray,flying}$	Local emission from spray and wash-off	[kg.d-1]	O
$C_{spray,wall,wash-off,soil}$	Local concentration of a.i. due to wash-off	[kg.kg_{ww}-1]	O
$C_{spray,flying,soil}$	Local concentration of a.i. due to wash-off/spray	[kg.kg_{ww}-1]	O

Table III-158 Default values for the application step of the outdoor spray applications - flying insects

parameter	value
$AREA_{wall}$	Private house (125), public/industrial building (625)
$F_{spray,wall}$	0.3
$F_{spray,wash-off}$	0.5
$V_{spray,soil}$	Private house (13), public/industrial building (63)
RHO_{soil}	1700

Total release

$$E_{total} = ((E_{spray})_{house} \cdot N_{houses} + (E_{spray})_{building} \cdot N_{building}) \cdot F_{simultaneity} \qquad \textbf{(549)}$$

Input		
E_{spray}	Emission from spraying to waste water	[kg.d-1]
Nhouses	Number of houses by STP	[-]
Nbuilding	Number of buildings by STP	[-]
$F_{simultaneity}$	Simultaneity factor	[-]
Output		
E_{total}	Total Emission to waste water	[kg.d-1]

Table III-159 Default values for the application step of the outdoor spray application

parameter	value
N_{houses}	4000
$N_{building}$	1000
$F_{simultaneity}$	0.03

Outdoor Spray applications - crawling insects (18.3.2)

Mixing / loading step

See spray application – flying insects.

Application step

Parameters/variables and default values for application step of outdoor spray application of crawling insects.

$$E_{spray,\,foundation} = Q_{prod} \cdot F_{ai} \cdot AREA_{foundation} \cdot F_{spray,\,foundation} \qquad \textbf{(550)}$$

$$E_{spray,soil} = AREA_{soil} \cdot Q_{prod} \cdot F_{ai} \cdot F_{spray,soil} \qquad \textbf{(551)}$$

Emission Rural : soil; urban: STP

Input			
Q_{prod}	Quantity of product applied	[kg.m-2]	S
F_{AI}	Fraction of active substance in the commercial product	[-]	S
$AREA_{foundation}$	Area of foundation treated per day	[m2.d-1]	P
$AREA_{soil}$	Area of soil treated per day	[m2.d-1]	P
$F_{spray,foundation}$	Fraction emitted to soil during application	[-]	D
$F_{spray,soil}$	Fraction emitted to soil during application	[-]	P
$F_{spray,untreatedsoil}$	Fraction emitted to untreated soil	[-]	P
$V_{spray,treatedsoil}$	Treated soil volume	[m3]	P
$V_{spray,untreatedsoil}$	Untreated soil volume	[m3]	P
RHO_{soil}	Bulk density of wet soil	[kg_{ww}.m-3]	D
Output			
$E_{spray,foundation}$	Emission from spraying on foundation	[kg.d-1]	O
$E_{spray,soil}$	Emission from spraying to soil	[kg.d-1]	O
$E_{spray,untreatedsoil}$	Emission from spraying to untreated soil	[kg.d-1]	O
$C_{spray,treatedsoil}$	Concentration of a.i. in treated soil	[kg.kg_{ww}-1]	O
$C_{spray,untreatedsoil}$	Concentration of a.i. in untreated soil	[kg.kg_{ww}-1]	O

Wash-off of the treated surface by rainfall

$$E_{spray,\,foundation,wash-off} = AREA_{foundation} \cdot Q_{prod} \cdot F_{ai} \cdot F_{spray,wash-off} \qquad \textbf{(552)}$$

Emission rural: soil; urban: STP

Urban area

$$E_{spray,\,foundation,wash-off} = E_{spray,\,foundation} + E_{spray,soil} + E_{spray,\,foundation,wash-off} \qquad \textbf{(553)}$$

Emission to STP

Rural area (treated)

$$C_{spray,treated,soil} = \frac{E_{spray,\,foundation} + E_{spray,soil} + E_{spray,\,foundation,wash-off}}{V_{spray,treatedsoil} \cdot RHO_{soil}} \qquad \textbf{(554)}$$

Emission to soil

Rural area (untreated)

$$C_{spray,untreated,soil} = \frac{E_{spray,untreatedsoil}}{V_{spray,untreatedsoil} \cdot RHO_{soil}} \qquad \mathbf{(555)}$$

Emission to soil

Input			
Q_{prod}	Quantity of product applied	[kg.m-2]	S
F_{AI}	Fraction of active substance in the commercial product	[-]	S
$AREA_{foundation}$	Area of foundation treated per day	[m2.d-1]	P
$F_{spray,wash-off}$	Fraction emitted to soil due to wash-off by rainfall	[-]	D
$V_{spray,treatedsoil}$	Soil volume for the wash-off at 0.5 m (treated)	[m3]	D
RHO_{soil}	Bulk density of wet soil	[kg_{ww}.m-3]	D
Output			
$E_{spray,foundation,wash-off}$	Local emission from spray on foundation	[kg.d-1]	O
$C_{spray,wall,wash-off}$	Local concentration of a.i. due to wash-off	[kg.kg_{ww}-1]	O
$C_{spray,treatedsoil}$	Local concentration of a.i. in treated soil	[kg.kg_{ww}-1]	O
$C_{spray,untreatedsoil}$	Local concentration of a.i. in untreated soil	[kg.kg_{ww}-1]	O

Table III-160 Default values for the application step of the outdoor spray applications - crawling insects

parameter	**value**
$AREA_{foundation}$	Private house (25), public/industrial building (125)
$AREA_{soil}$	Private house (26), public/industrial building (126)
$F_{spray,foundation}$	0.3
$F_{spray,soil}$	0.97
$F_{spray,untreatedsoil}$	0.03
$F_{spray,wash-off}$	0.5
$V_{spray,treatedsoil}$	Private house (13), public/industrial building (63)
$V_{spray,untreatedsoil}$	Private house (14), public/industrial building (64)
RHO_{soil}	1700

Total release

The calculation method is *mutatis mutandis* the same as used for spray application.

Outdoor Crawling space application (18.3.3)

Mixing / loading step

See spray application – flying insects.

Application step

Parameters/variables and default values for application step of outdoor crawling space application.

$$E_{crawling,soil} = Q_{prod} \cdot F_{ai} \cdot ((AREA_{crawling} \cdot F_{spray,wall-ceiling}) + (AREA_{house} \cdot F_{spray,soil}) \qquad \textbf{(556)}$$

$$C_{crawling,soil} = \frac{E_{crawling,soil}}{V_{spray,treatedsoil} \cdot RHO_{soil}} \qquad \textbf{(557)}$$

Emission Rural : soil; urban: STP

Input			
Q_{prod}	Quantity of product applied	[kg.m-2]	S
F_{AI}	Fraction of active substance in the commercial product	[-]	S
$AREA_{crawling}$	Area of crawling space treated per day	[m2.d-1]	D/S
$AREA_{house}$	Area of soil treated per day	[m2.d-1]	P/S
$F_{spray,wall-ceiling}$	Fraction emitted to soil during application on walls	[-]	D
$F_{spray,soil}$	Fraction emitted to soil during application on soil	[-]	D
$V_{spray,treatedsoil}$	Soil volume for deposition and application	[m3]	P/S
RHO_{soil}	Bulk density of wet soil	[kg_{ww}.m-3]	D
Output			
$E_{crawling,soil}$	Emission from crawling space spray application to soil	[kg.d-1]	O
$C_{crawling,soil}$	Concentration of active ingredient in soil	[kg.kg_{ww}-1]	O

Table III-161 Default values for the application step of the outdoor applications - Spray application – Crawling space application

parameter	**value**
$AREA_{crawling}$	Private house (156), public/industrial building (-)
$AREA_{house}$	Private house (131), public/industrial building (-)
$F_{spray,wall-ceiling}$	0.3
$F_{spray,soil}$	1
$V_{spray,treatedsoil}$	Private house (65), public/industrial building (-)
RHO_{soil}	1700

Total release

The calculation method is *mutatis mutandis* the same as used for spray application.

Outdoor nest spray application (18.3.4)

Mixing / loading step

See spray application – flying insects.

Application step

Parameters/variables and default values for application step of outdoor nest spray application.

$$E_{spra,nest,soil} = Q_{prod} \cdot F_{ai} \cdot F_{spray,nest,deposition} \qquad \textbf{(558)}$$

$$C_{spray,nest,soil} = \frac{E_{spray,nest,soil}}{V_{spray,,nest,soil} \cdot RHO_{soil}} \qquad \textbf{(559)}$$

Input			
Q_{prod}	Quantity of product applied	[kg]	S
F_{AI}	Fraction of active substance in the commercial product	[-]	S
$F_{spray,nest,deposition}$	Fraction emitted to soil during nest spray application	[-]	D
$V_{spray,nest,soil}$	Soil volume for deposition and application	[m3]	D
RHO_{soil}	Bulk density of wet soil	[kg$_{ww}$.m-3]	D
Output			
$E_{spray,nest,soil}$	Emission to soil during nest spray application	[kg.d-1]	O
$C_{spray,nest,soil}$	Concentration of active ingredient in soil	[kg.kg$_{ww}$-1]	O

Table III-162 Default values for the application step of the outdoor nest spray applications

parameter	**value**
$F_{spray,nest,soil}$	0.1
RHO_{soil}	1700

Outdoor spot application

Mixing / loading step

See spray application – flying insects.

Application step

Parameters/variables and default values for application step of outdoor spot application.

$$E_{spot,soil} = Q_{prod} \cdot F_{ai} \cdot N_{sites} \cdot N_{appl} \cdot F_{spot,soil} \qquad \textbf{(560)}$$

($F_{spot,soil}$ can be equal to $F_{spot,gel}$, $F_{spot,bait}$ or $F_{outdoor,nestpowder,soil}$)

$$C_{spot,soil} = \frac{E_{spot,soil}}{AREA_{exposed} \cdot DEPTH_{soil} \cdot RHO_{soil}} \quad \textbf{(561)}$$

Input

Q_{prod}	Quantity of product applied	[g]	S
F_{AI}	Fraction of active substance in the commercial product	[-]	S
N_{sites}	Number of application sites	[-]	S
N_{appl}	Number of applications	[-]	S
$F_{spot,gel}$	Fraction emitted to STP during outdoor gel application	[-]	D
$F_{spot,bait}$	Fraction emitted to STP during outdoor bait application	[-]	D
$F_{outdoor,nestpowder,soil}$	Fraction emitted to STP during powder application	[-]	D
$AREA_{exposed}$	Area directly exposed to insecticide	[m2]	D/S
$DEPTH_{soil}$	Depth of exposed soil	[m]	D
$VOLUME_{soil}$	Volume of exposed soil	[m3]	D/S
RHO_{soil}	Bulk density of wet soil	[kg.m-3]	D
Output			
$E_{spot,soil}$	Direct emission rate of a.i. to soil from a campaign	[g]	O
$E_{spot,air}$	Direct emission rate of a.i. to air from a campaign	[g]	O
$C_{spot,soil}$	Local concentration in soil due to release after a campaign	[mg.kg-1]	O

Table III-163 Default values for the application step of the outdoor spot application

parameter	**value**
$F_{spot,gel}$	0.9
$F_{spot,bait}$	0.2
$F_{outdoor,nestpowder,soil}$	0.9
$AREA_{exposed}$	Single point of release (0.25), other (-)
$DEPTH_{soil}$	0.5
$VOLUME_{soil}$	Single point of release (0.125), other (-)
RHO_{soil}	1700

Total release

The calculation method is *mutatis mutandis* the same as used for spray application.

Secondary poisoning

Parameters/variables and default values for the estimated daily intake calculations for the risk assessment of exposure of contaminated food to predators

$$APPL_{ground} = Q_{prod} * F_{AI} \quad \textbf{(562)}$$

$$ETE_{acute,crwaling} = (FIR/bw) \cdot RUD \cdot APPL_{ground} \cdot 1.15 \cdot 10^{4} \quad \textbf{(563)}$$

$$ETE_{short-term,insectivorous,flying} = (FIR/bw) \cdot RUD_{mean} \cdot APPL_{ground} \cdot 2.5 \cdot 10^{4} \quad \textbf{(564)}$$

$$ETE_{short-term,insectivorous,crwaling} = (FIR/bw) \cdot RUD_{mean} \cdot APPL_{ground} \cdot 1.5 \cdot 10^{4} \qquad \textbf{(565)}$$

$$ETE_{short-term,herbivorous,flying} = (FIR/bw) \cdot RUD_{mean} \cdot APPL_{ground} \cdot 2.5 \cdot 10^{4} \cdot MAF \qquad \textbf{(566)}$$

$$ETE_{short-term,herbivorous,crwaling} = (FIR/bw) \cdot RUD_{mean} \cdot APPL_{ground} \cdot 1.5 \cdot 10^{4} \cdot MAF \qquad \textbf{(567)}$$

$$ETE_{acute,worm,mammal} = 1.4 \cdot C_{worm,applicationsoil} \qquad \textbf{(568)}$$

$$ETE_{short-term,worm,mammal} = 1.4 \cdot C_{worm,spray,wall/foundation+wall/spray,wall/foundation,wash-off} \qquad \textbf{(569)}$$

$$ETE_{acute,worm,bird} = 1.1 \cdot C_{worm,applicationsoil} \qquad \textbf{(570)}$$

$$ETE_{short-term,worm,bird} = 1.1 \cdot C_{worm,spray,wall/foundation+wall/spray,wall/foundation,wash-off} \qquad \textbf{(571)}$$

$$C_{worm} = \frac{BCF \cdot C_{porewater} + C_{soil} \cdot F_{gut} \cdot CONV_{soil}}{1 + F_{gut} \cdot CONV_{soil}} \qquad \textbf{(572)}$$

$$CONV_{soil} = \frac{RHO_{soil}}{F_{soilid} \cdot RHO_{soil}} \qquad \textbf{(573)}$$

Input			
C	Concentration of substance in fresh diet	[mg.kg-1]	
FIR	Food intake rate of indicator species	[g .d-1]	S/P
bw	Body weight	[g]	S/D
AV	Avoidance factor	[-]	S/D
PT	Fraction of diet obtained in treated area	[-]	S/D
PD	Fraction of food type in diet	[-]	S/D
Q_{prod}	Quantity of commercial product applied	[kg.m-2]	S
F_{AI}	Fraction of active substance in the commercial product	[-]	S
RUD	Residue value per unit dose	[mg.kg-1]	S/P
T_{appl}	Application rate of active substance	[kg.m-2]	S
MAF	Multiple Application Factor	[-]	S
Output			
ETE	Estimated daily uptake of a compound	[mg.kg-1.d-1]	O

AV, PD and PT are all set to 1 and are therefore not included in the calculations

Table III-164 *:* Indicator species representative of the lawn/garden and relevant for secondary poisoning

Indicator species	Example – species	Main food type/ category	Body weight
Small insectivorous mammal 1 (a)	Pipistrelle	Large insects	7.6 g
Small insectivorous mammal 2 (b)	Shrew	Large insects/earthworms	10 g
Small insectivorous mammal 3 (a)	Mole	Worms & slugs	85 g
Medium insectivorous mammal (a)	Hedgehog	Large insects/ Worms & slugs	1,100 g
Large insectivorous mammal (a)	Badger	Large insects/ Worms & slugs	10,100 g
Small herbivorous mammal (c)	Vole	Grasses	25 g
Medium herbivorous mammal (a)	Rabbit	Leafy plants	1,500 g
Small Insectivorous bird 1 (c)	Wren, tit	Small insects	10 g
Small Insectivorous bird 2 (a)	Tree sparrow, robin	Small insects	22 g
Medium Insectivorous bird (a)	Blackbird	Earthworms/ insects	113 g
Omnivorous bird (d)	Black-billed Magpie	80% animal matter (insects, small mammals…)	225 g
Medium herbivorous bird (c)	Partridge, pigeon	Leafy plants	300 g
Large herbivorous bird (c)	Goose	Short grasses	3,000 g

(a) Indicator species assumed to be relevant for lawn/garden and not considered as indicator species in (SANCO/4145 2002). Data from (Crocker *et al.* 2002) except for black-billed magpie.

(b) Indicator species considered relevant for cereals crop in (SANCO/4145 2002)

(c) Data from (SANCO/4145 2002)

(d) Data from (Thomas 1994)

Table III-165 *:* Food intake rate (FIR) for indicator species of lawn/garden with parameters referenced in (Crocker et al. 2002)

Indicator species	**Daily Energy Expenditure [1] (kj/d)**	**Food characteristic [2]**			**Assimilation efficiencies [3] (%)**	**FIR [4] (fresh materiel) (g/day)**
		Food type	*Energy (kJ/g dry wgt)*	*Moisture (%)*		
Small insectivorous mammal 1 - Pipistrelle (7.6 g)	29.3	Arthropods	21.9	70.5	88	5.2
Small insectivorous mammal 3 – Mole (85 g)	160.9	Soil invertebrates	19.3	84.6	88	61.2
Medium insectivorous mammal – Hedgehog (1100 g)	978.6	Arthropods	21.9	70.5	88	172.1
		Soil invertebrates	19.3	84.6	88	374.2
Large insectivorous mammal – Badger (10100 g)	4673.1	Arthropods	21.9	70.5	88	822
		Soil invertebrates	19.3	84.6	88	1786.7
Medium herbivorous mammal – Rabbit (1500 g)	1217.9	Grasses, cereal shoots	18	76.4	74	387.4
Small Insectivorous bird 2 - Tree sparrow, robin (22 g)	88.4	Arthropods	21.9	70.5	76	18
Medium Insectivorous bird – Blackbird (113 g)	196.7	Soil invertebrates	19.3	84.6	76	87.1
Omnivorous bird - Black-billed Magpie (225 g)	453.8	Arthropods	21.9	70.5	76	92.4
		Soil invertebrates	19.3	84.6	76	200.9

1) DEE calculated from “other eutherians” equation and “passerine” equation for mammals and birds respectively (see Tables 1/2 in *Crocker et al*., 2002)

2) values from *Crocker et al*. (2002) in Table 4

3) values from *Crocker et al*. (2002) in Tables 5/6

4) with FIR = DEE / ((Energy in food × (1-Moisture) × Assimilation on efficiency)).

Table III-166 : Food intake rates per body weight (FIR/bw) for indicator species and residues values in contaminated vegetation and insects (normalised for an application rate of 1 kg active ingredient/ha)

Indicator species – body weight	Category	FIR/bw	RUD	
			Acute (90%)	*Short-term (mean)*
Small insectivorous mammal 1 (pipistrelle) – 7.6 g *	Large insects	0.68	14	5.1
Small insectivorous mammal 2 - 10 g	Large insects	0.63	14	5.1
Medium insectivorous mammal – 1100 g – hedgehog *	Large insects	0.18	14	5.1
Large insectivorous mammal – 10100 g (badger) *	Large insects	0.18	14	5.1
Small herbivorous mammal – 25 g	Short grass	1.39	142	76
Medium herbivorous mammal – 1500 g (rabbit) *	Leafy crops	0.32	87	40
Small Insectivorous bird 1 – 10 g	Small insects	1.04	52	29
Small Insectivorous bird 2 (Tree sparrow, robin) – 22 g	Small insects	0.2	52	29
Medium Insectivorous bird – 113 g (blackbird) *	Large insects	0.44	14	5.1
Omnivorous bird – 225 g (magpie) *	Large insects	0.2	14	5.1
Medium herbivorous bird – 300 g	Leafy crops	0.76	87	40
Large herbivorous bird – 3000 g	Short grass	0.44	142	76

*Indicator species considered as relevant for lawn/garden

Table III-167 : Multiple Application Factors in acute and short-term exposures for residues on vegetation (SANCO/4145 2002)

Interval (days)	Number of applications											
	2		**3**		**4**		**5**		**6**		**8**	
	Acute	*Short-term*	*Acute*	*Short-term*	*Acute*	*Short-term*	*Acute*	*Short-term*	*Acute*	*Short-term*	*Acute*	*Short-term*
7	1.4	1.6	1.7	2.0	1.8	2.2	1.9	2.4	1.9	2.5	2.0	2.5
10	1.3	1.5	1.5	1.8	1.6	1.9	1.6	1.9	1.6	2.0	1.6	2.0
14	1.2	1.4	1.3	1.5	1.4	1.6	1.4	1.6	1.4	1.6	1.4	1.6

III.3.6.15 Product type 21: Antifouling products

The scenarios and models and calculation formulations used in this version of EUSES 2.1.1 for antifouling products have been taken from the following document:

- Harmonisation of Environmental Emission Scenarios: An Emission Scenario Document for Antifouling Products in OECD countries. (EC, Directorate-General Environment, 2004)

This document can be obtained from the ECB Biocides website

The following additions are made:
The ESD provides formulas to calculate the total emissions to the different compartments only, but not to calculate the concentrations. In the present EUSES 2.1.1 version formulas are implemented taken into account the possibility for (bio)degradation and using the dimensions given in the ESD. These formulas are based on those given in the USES 2.0 documentation, section III 4.9.1 and 4.8.16 (Linders and Jagers, 1998).

.3.5.3. Antifouling

The following scenarios for calculation the concentration in different environmental compartments for the application and removal of compounds used as antifoulings can be distinguished:

New building

- Commercial ships professional (scenario 1);
- Pleasure craft professional. (scenario 2)

Maintenance and repair

- Commercial ships professional (scenario 3);
- Pleasure craft professional (scenario 4);
  non-professional (scenario 5).

The scenarios for new building are related to the application of an antifouling paint only. Removal of the old paint layer on a ship hull takes place only during M&R of ship hulls after which a new paint will be applied.
It is considered that application and removal for the maintenance and repair occur within the same time frame and at the same site. Therefore, the emissions from application and removal have to be linked to one other. With respect to the emission to soil this means that the calculated PECs will be summed up. With respect to the release to STP and/or water, the PECs can be treated separately, assuming that the time between application and removal is long enough for a total dissipation/dilution.

For most of the scenario the direct emission is restricted to one or two compartments:

New building

• Commercial ships	professional	water
• Pleasure craft	professional.	soil, STP

Maintenance and repair

• Commercial ships	professional;	water
• Pleasure craft	professional;	soil, STP (and water at removal only)
	non-professional.	soil, STP (and water at removal only)

Overview of the timeframe for application and removal of paint

Application

New building ships (emission to water)

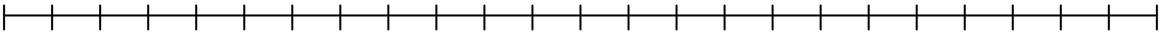
Tfreq = 2 (2 days per year a ship will be painted)

Tpaint = 1 day	Tpaint = 1 day
Nboat = 1	Nboat = 1

The PEC in water and sediment (via EP) will be calculated on a daily base both for a river and a harbour.

New building pleasure craft (emission to soil and STP)

Realistic worst case: Tfreq = 30 with regular intervals (Total painting days = 2 * 30 days)
Typical case is different: Tpaint = 365 and Nboat = 300, hence all most every days a pleasure craft is painted. However, according to the ESD there is no emission.



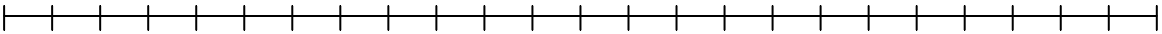
Tpaint = 2 days
Nboat = 1

The concentration in water and sediment (via EP) resulting from the release to a STP will be calculated on a daily base.
The concentration in sludge will be divided by 6.1 (=365/60) to calculate a yearly average sludge concentration.
The concentration in soil will be calculated using the equations 1 -6, where $Csoil_{paint-0}$ is based on two paint days.

Application of paint and removal

M&R ships (emission to water)

Realistic worst case and typical case: Tfreq = 20 with regular intervals (Total painting days = 2 * 20 days)

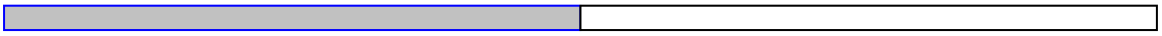


Tpaint = 2 days
Tremoval = 1 day
Nboat = 1

The PEC in water and sediment (via EP) in a harbour will be calculated based on two painting days and 1 removal day, taking into account removal process between these events (see P-8)
It is assumed that the interval between the different painting + removal events is long enough that no accumulation is to be expected.
The PEC water and sediment in a river will be calculated on a daily base.

M&R pleasure craft (prof) (emission to soil and STP+ water with respect to removal)

The calculated Elocal to soil and STP are daily emissions during a period of 183 days, after which no activities take place during 183 days (Total painting days = 183 days)



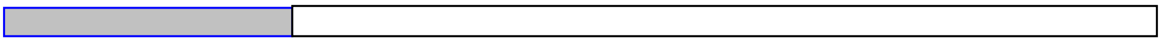
Tpaint = 183 days Tint = 183 days

The concentration in water and sediment (via EP) resulting from the release to a STP will be calculated on a daily base. As the release is continuous no deviation from the standard calculation of the concentration in sludge is necessary. The concentration in sludge for application and removal has to be added.
The concentration in soil will be calculated using the equations 1 -6, where $Csoil_{paint\text{-}0}$ is based on a daily release.

M&R pleasure craft (non-prof) (emission to soil and STP+ water with respect to removal)

At this scenario 5 boats are painted within a period of 91 days with regular intervals (Tinterval = 91/(5-1)= 22.5 days). Total painting days = 1 * 5 days

For removal there are two scenarios typical and realistic worst case. For typical case the same scenario is used as for application.
For realistic worst case every day (during 91 days) paint is removed.



Tpaint = 91 days Tint = 274 days

Nboat = 5

Ndays = 1 (days to paint a craft)

The concentration in water and sediment (via EP) resulting from the release to a STP will be calculated on a daily base.
The concentration in sludge will be divided by 18.2 (=91/5) to calculate an average sludge concentration.

As the release is continuous no deviation from the standard calculation of the concentration in sludge is necessary
The concentration in soil will be calculated using the equations 1 -6, where $Csoil_{paint\text{-}0}$ is based on a daily release.

III.3.6.15.1 New building commercial ships

Intermediate calculations:

$$\mathrm{Vpaint} = Ncoats \cdot \frac{\mathrm{AREAship}}{\mathrm{Coverage}} \qquad \textbf{(574)}$$

$$\mathrm{E}\mathit{localwater} = \frac{\mathrm{Vpaint} \cdot \mathrm{Nship} \cdot \mathrm{Fwater} \cdot \mathrm{Ca.i}}{\mathrm{Tpaint}} \qquad \textbf{(575)}$$

Input

Tpaint	The painting period	[d]	D
Nship	Number of ships treated per painting period	[-]	D
AREAship	The average hull surface of a ship	[m2]	D
COVERAGE	Theoretical coverage of the paint	[m2.l-1]	S
Ncoats	Number of coats applied on the hull [-]	D	
Ca.i.	The concentration of a.i. in the paint [g.l-1]	S	
Fwater	Fraction to surface water	[-]	D

Intermediate results

Vpaint	The theoretical amount of paint applied per ship	[l]	O
Elocalwater	Total emission to surface water	[g.d-1]	O

End calculation

$$Clocalwater_{harbour} = \frac{\mathrm{Elocalwater}}{\mathrm{LENGTHch} \cdot \mathrm{WIDTHch} \cdot \mathrm{DEPTHch}} \qquad \textbf{(576)}$$

$$Clocalwater_{river} = \frac{\mathrm{Elocalwater}}{\mathrm{Debwater}} \qquad \textbf{(577)}$$

Input

Tfreq	The painting frequency per year	[-]	D
LENGTHch	Length of the harbour	[m]	D
WIDTHch	Width of the harbour	[m]	D
DEPTHch	Depth of the harbour	[m]	D

Dedriver	Debite of a river	[m3.d-1]	S
Output			
PEClocalwater	Predicted environmental concentration in surface water	[g.m-3]	O

Table III-168 Default setting new building ships in an average OECD shipyard: application of paint

Variable/parameter	Symbol	Unit	Value for realistic worst case	Value for typical case
The painting period	Tpaint	[d]	$1^{1)}$	$1^{1)}$
Number of ships treated in an EU/US shipyard per painting period	Nship	[-]	1	1
The average hull surface of a ship	AREA$_{ship}$	[m^2]	EU/US: 2500 Asia: $8600^{2)}$	EU/US: 2500 Asia: $8600^{2)}$
Theoretical coverage of the paint	COVERAGE	[m^2.l^{-1}]		
Number of coats applied on the hull	Ncoats	[-]	1 (only the final coat)	1 (only the final coat)
Fraction to surface water	F$_{water}$	[-]	$0.35^{3)}$	0.075
Fraction to soil	F$_{soil}$	[-]	0	0
The painting frequency per year$^{5)}$	Tfreq	[-]	2	
Length of the harbour	LENGTHch	[m]	5000	
Width of the harbour	WIDTHch	[m]	1000	
Depth of the harbour	DEPTHch	[m]	15	

1) Expert judgement: 1 day is needed for the application of the final coat (expert judgement CEPE). The application of the first coat is not included in this scenario.

2) Note that all other values are based on the European/US situation.

3) Note that this fraction seems fairly high. It would mean that a third of the antifouling paint ends up in the water. This fraction is derived from Safinah (2004): potential emission based on overspray during application of the paint on a slipway. The fraction of 0.35 is also described as the realistic worst case loss factor for airless spray in the RIVM comments. According to Finnish data the total losses are typically 30% of the total amount of paint used which would result in 0.43 as a sum of all these emission fractions (water, soil, STP, waste).

4) The theoretical paint demand is the amount of paint that is theoretically needed to paint the entire ship hull. The theoretical paint demand does not contain the excess paint applied on the hull due to overlap during the application process, the subsequent coating of join up seams and butts, etc. The theoretical paint demand and the excess paint together form the total amount of paint that is applied on the ships hull

5) The amount of painting periods per year.

III.3.6.15.2 New building pleasure craft (professional)

Intermediate calculations:

$$Elocal_{soil} = \frac{\mathrm{Vpaint} \cdot \mathrm{Nboat} \cdot \mathrm{F_{soil}} \cdot \mathrm{Ca.i}}{\mathrm{Tpaint}} \qquad \textbf{(578)}$$

$$Elocal_{STP} = \frac{\mathrm{Vpaint} \cdot \mathrm{Nboat} \cdot \mathrm{F_{STP}} \cdot \mathrm{Ca.i}}{\mathrm{Tpaint}} \qquad \textbf{(579)}$$

Input			
Tpaint	The painting period	[d]	D
Nboat	Number of boats treated per painting period	[-]	D
Vpaint	The theoretical amount of paint applied per boat	[l]	D
Ca.i.	The concentration of a.i. in the paint [g.l-1]	S	
F_{soil}	Fraction to soil	[-]	D
F_{STP}	Fraction to STP	[-]	D
Intermediate results			
Elocalsoil	Total emission to soil	[g.d-1]	O
ElocalSTP	Total emission to STP	[g.d-1]	O

End calculation

Soil

$$Clocalsoil_{appli-1} = \frac{\mathrm{Elocal_{soil}} \cdot \mathrm{Tpaint}}{\mathrm{LENGTHch} \cdot \mathrm{WIDTHch} \cdot \mathrm{DEPTHch} \cdot \mathrm{RHOsoil}} \qquad \textbf{(580)}$$

For those scenarios where releases to soil will occur, accumulation of the active substance after several application/removals has to be considered. Therefore, the maximum concentration, reached during this period, should be calculated. Assuming only first order biodegradation this concentration can be calculated as the concentration after one application/removal plus the remaining contributions from earlier applications/removals. The result depends on the half-life for biodegradation, the application/removal frequency, and the interval between two applications/removals.

The initial Predicted Environmental Concentration is set at this maximum concentration during the application/removal period. This PEC is considered to be equal to the concentration on day 0 ($Cloca_{-0}$), which is used in several models.

$$F_{rs} = e^{-kdeg_{soil} \cdot T_{\text{interval}}} \tag{581}$$

$$T_{interval} = \frac{T_{paint/removal}}{T_{freq-1}}$$

$$\begin{aligned} \mathrm{Csoil}_{\mathrm{appl/removal\text{-}0}} &= \mathrm{Csoil}_{\mathrm{appl/remov}} + \mathrm{Csoil}_{\mathrm{appl/remov}} \cdot \mathrm{F}_{\mathrm{rs}} + \\ &\quad \mathrm{Csoil}_{\mathrm{appl/remov}} \cdot \mathrm{F}_{\mathrm{rs}}^{2} + \ldots + \mathrm{Csoil}_{\mathrm{appl/remov}} \cdot \mathrm{F}_{\mathrm{rs}}^{(\mathrm{N}_{\mathrm{appl/remov}} - 1)} \\ &= \mathrm{Csoil}_{\mathrm{appl/remov}} \cdot \frac{1 - \mathrm{F}_{\mathrm{rs}}^{\mathrm{N}_{\mathrm{appl}}}}{1 - \mathrm{F}_{\mathrm{rs}}} \end{aligned} \tag{582}$$

Input			
LENGTHch	Length of the soil	[m]	D
WIDTHch	Width of the soil	[m]	D
DEPTHch	Depth of the soil	[m]	D
$RHOsoil_{dwt}$	Soil density (dry weight)	$[kg.m^{-3}]$	D
$Csoil_{paint\text{-}1\ appl}$	concentration in soil after one application/removal	$[kg_{c}.kg_{wwt}^{-1}]$	O
$kdeg_{soil}$	rate constant for degradation in soil	$[d^{-1}]$	O
N_{appl}	number of applications/removal in one year	[-]	D
F_{rs}	fraction of the concentration remaining after time $T_{interval}$	[-]	O^{c}
$T_{interval}$	application interval	[d]	D
T_{paint}	the painting period	[d]	D
T_{freq}	the painting frequency per year	[-]	D
Output			
$Csoil_{paint\text{-}0}$	peak concentration in soil after *N* applications	$[kg_{c}.kg_{wwt}^{-1}]$	O
$Csoil_{paint\text{-}T}$	average in soil concentration over *T* days	$[kg_{c}.kg_{wwt}^{-1}]$	O

PECs for soil, long-term application

The PEC after long-term application is set at the concentration after the last application/removal in the tenth year. This PEC is considered to be equal to the soil concentration at year 10 ($Csoil_{paint\text{-}0,lt}$). After the tenth year the resulting concentration, $Csoil_{paint\text{-}lt}$, is compared to the PNEC.

$$\mathrm{Csoil}_{\mathrm{paint}-1} = \mathrm{Csoil}_{\mathrm{paint}-0} \cdot \mathrm{e}^{-\ \mathrm{kdeg}_{\mathrm{soil}} \cdot (365 - \mathrm{T}_{\mathrm{paint}})} \tag{583}$$

$$F_{lt} = \frac{Csoil_{paint-1}}{Csoil_{paint-0}} \tag{584}$$

Peak concentration at last application/removal:

$$Csoil_{paint/removal\text{-}0,lt} = Csoil_{paint/removal\text{-}1} + Csoil_{paint/removal\text{-}1} \cdot F_{lt} +$$

$$Csoil_{paint/removal\text{-}1} \cdot F_{lt}^{2} + \ldots + Csoil_{paint/removal\text{-}1} \cdot F_{lt}^{(N_{lt}-1)} \tag{585}$$

$$= Csoil_{paint/removal\text{-}1} \cdot \frac{1 - F_{lt}^{N_{lt}}}{1 - F_{lt}}$$

Input			
$Csoil_{paint\text{-}1}$	concentration in soil after one year,	$[kg_c.kg_{wwt}^{-1}]$	O
N_{lt}	number of application periods per registration period	[-]	S
$T_{interval\text{-}lt}$	long term interval for application periods	[d]	S
F_{lt}	fraction of the concentration remaining after one year	[-]	O^c
$Csoil_{paint\text{-}1}$	concentration in soil after 1 year	$[kg_c.kg_{wwt}^{-1}]$	O^c
$Csoil_{paint\text{-}0}$	peak concentration in soil after 1 year	$[kg_c.kg_{wwt}^{-1}]$	O^c
Output			
$Csoil_{paint\text{-}0,lt}$	peak concentration in soil after N_{lt} years	$[kg_c.kg_{wwt}^{-1}]$	O^c

STP

Clocalwater is calculated by using the standard STP model
Csludge is calculated using the standard STP model divided by 6.1 to calculate a yearly average

Table III-169 New building pleasure craft in an average OECD boatyard: application of paint

Variable/parameter	**Symbol**	**Unit**	**Value for realistic worst case**	**Value for typical case**
The painting period	Tpaint	[d]	2	365
Number of boats treated in a boatyard per painting period	Nboat	[-]	1	300
The concentration of active ingredient in the paint	Ca.i.	[$g.l^{-1}$]		
The theoretical amount of paint applied per boat[1]	Vpaint	[l]	3	3
Fraction to surface water	F_{water}	[-]	0	0
Fraction to STP[2]	F_{STP}	[-]	Application by mixture of airless spray / brush and roller: Max. 0.06 Application by brush and roller only: Max. 0.025	0
Fraction to soil[2]	F_{soil}	[-]	Application by mixture of airless spray / brush and roller: Max. 0.06 Application by brush and roller only: Max. 0.025	0
The painting frequency per year	Tfreq	[-]	Realistic worst case: 30 Typical case: n/a	
Length of the receiving soil compartment[3]	LENGTH	[m]	9.5	9.5
Width of the receiving soil compartment	WIDTH	[m]	4.5	4.5
Depth of the receiving soil compartment	DEPTH	[m]	0.1[4]	0.1[4]
Soil density (dry weight)	$RHOsoil_{dw}$	[$kg.m^{-3}$]	1504[5]	1504[5]

1) The system of paint volume demand is very different to ships. Most of the paint companies assume that the coating will be applied by the boat owner/yard and so supply a paint calculator. Using this calculator the required paint amount can be estimated. However, this is not what happens in practice. In reality the typical owner applies one touch up coat to the existing antifouling coating and one full coat of antifouling. On the basis of discussions with paint companies, boat builders and marina operators etc. Safinah has determined default values for the theoretical amount of paint applied per boat.

2) Depending on the control measurements of the boat yard the emission up to a maximum of 6% (potential emission weighted for brush/roller and spray) or 2.5% (for brush and roller only) either goes to soil or a STP or a mixture between these two options

3) A boat of 7.5 m length and 2.5 m width is assumed. For the determination of the surface of the receiving soil compartment a “walking path” around the boat for the applier of the paint is assumed. It was estimated that this path is 1 metre wide.

4) In line with the environmental emission scenario of the OECD for Wood Preservatives.

5) Based on EU-TGD (ECB, 20034) (wet weight is 1700 $kg.m^{-3}$).

III.3.6.15.3 Maintenance and repair

- Commercial ships professional;

Application

$$\mathrm{Vpaint} = Ncoats \cdot \frac{\mathrm{AREAship}}{\mathrm{Coverage}} \qquad \textbf{(586)}$$

$$\mathrm{E}localwater = \frac{\mathrm{Vpaint} \cdot \mathrm{Nship} \cdot \mathrm{Fwater} \cdot \mathrm{Ca.i}}{\mathrm{Tpaint}} \qquad \textbf{(587)}$$

Input

Tpaint	The painting period	[d]	D
Nboat	Number of boats treated per painting period	[-]	D
Vpaint	The theoretical amount of paint applied per boat	[l]	D
AREAship	The average hull surface of a typical OECD ship	[m2]	D
COVERAGE	Theoretical coverage of the paint	[m2.l-1]	S
Ncoats	Number of coats applied on the hull	[-]	D
Ca.i.	The concentration of a.i. in the paint [g.l-1]	S	
F_{water}	Fraction to surface water	[-]	D
Intermediate results			
Elocalwater	Total emission to surface water	[g.d-1]	O

Removal

$$\mathrm{Vpaint} = Ncoats \cdot \frac{\mathrm{AREAship}}{\mathrm{Coverage}} \cdot (1 + Fexcess) \tag{588}$$

$$\mathrm{E}localwater = \frac{(\mathrm{Vpainttotal} \cdot \mathrm{Nboat} \cdot \mathrm{Ca.i} \cdot (\mathrm{F}_{washing} \cdot \mathrm{Fa.iexh\ paint} + \mathrm{F}_{abrasion} \cdot \mathrm{Fa.i\ oldpaint}) \cdot \mathrm{F}_{water})}{\mathrm{Tremoval}} \tag{589}$$

Emission load for the calculation of the yearly average:

Elocalwater = (Vpainttotal * Nboat * Ca.i. * Fwater * (Fwashing * Fa.i.exhpaint + Fabrasion_reblasting * RATIOblasting * Fa.i.old paint + Fabrasion_spot blasting * Fa.i.old paint * (1-RATIOblasting))) /Tremoval **(590)**

Input

Tremoval	The removal period	[d]	D
Nboat	Number of boats treated per removal period	[-]	D
AREAship	The average hull surface of a typical OECD ship	[m2]	D
COVERAGE	Theoretical coverage of the paint	[m2.l-1]	S
Ncoats	Number of coats applied on the hull	[-]	D
Fexcess	Fraction excess paint applied	[-]	D
Fwashing	Fraction of the paint that is to be removed from the ships hull by HPW (exhausted paint)	[-]	D
Fabrasion	Fraction of the paint that is to be removed from the ships hull by abrasion	[-]	D
RATIOblasting	Ratio reblasting/spot blasting	[-]	
Ca.i.	The concentration of active ingredient in the original paint	[g.l-1]	S
Fa.i.exhpaint	Fraction of a.i. remained in exhausted paint removed by HPW	[-]	D
Fa.i.old paint	Fraction of a.i. remained in old paint removed by abrasion	[-]	D
Fwater	Fraction to surface water	[-]	D
Fsoil	Fraction to soil	[-]	D
Intermediate results			
Elocalwater	Total emission to surface water	[g.d-1]	O

End calculation

WATER

Harbour

$$Clocalwater_{harbour\ -appl/removal} = \frac{\mathrm{Elocalwater}}{\mathrm{LENGTHch} \cdot \mathrm{WIDTHch} \cdot \mathrm{DEPTHch}} \qquad \textbf{(591)}$$

$$Clocalwater_{harbour} = Cwater_{removal} \cdot e^{-k\,\mathrm{deg}_{ba\,\mathrm{sin}}.2.} + Cwater_{appl} \cdot e^{-k\,\mathrm{deg}_{ba\,\mathrm{sin}}.} + Cwater_{appli} \qquad \textbf{(592)}$$

River

Elocalwater goes directly to surface water. Therefore in EUSES by pass STP should be selected.

Here PEC water is calculated for application and removal separately. For the risk assessment the highest PEC is used.

Input

LENGTHch	Length of the harbour	[m]	D
WIDTHch	Width of the harbour	[m]	D
DEPTHch	Depth of the harbour	[m]	D
FLOWriver	Flow rate of a river	[$m^3.d^{-1}$]	S

Output

PEClocalwater	Predicted environmental concentration in surface water	[g.m-3]	O

parameters required for distribution models	**Default for this scenario**	**Unit**	**Value**
FLOW	$FLOW_{river}$	[$m^3.d^{-1}$]	-

Table III-170. Default setting for application of the paint layer in an average OECD shipyard

Variable/parameter	**Symbol**	**Unit**	**Value for realistic worst case**	**Value for typical case**
The painting period	Tpaint	[d]	2[1]	2[1]
Number of ships treated per painting period	Nboat	[-]	1	1
The average hull surface of a typical OECD ship	$AREA_{ship}$	[m^2]	EU/US: 2500 Asia: 7963[2]	EU/US: 2500 Asia: 7963[2]
Theoretical coverage of the paint	COVERAGE	[$m^2.l^{-1}$]		
Number of coats applied on the hull	Ncoats	[-]	2	2
Fraction to surface water	F_{water}	[-]	0.35	0.075[3]
Fraction to soil	F_{soil}	[-]	0	0

1) Expert judgement CEPE: one day for each coat.
2) Note that all other values are based on the European/US situation. Note also that the value for Asia is lower than for the new building scenario (Table 0.8) as also smaller ships are maintained and repaired.
3) See also application of paint during new building commercial ships.

Table III-171 Default setting for removal of the paint layer in an average OECD shipyard

Variable/parameter	**Symbol**	**Unit**	**Value for realistic worst case**	**Value for typical case**
Number of boats treated per removal period	Nboat	[-]	1 (as for application)	1 (as for application)
The average hull surface of a typical OECD ship	$AREA_{ship}$	[m^2]	EU/US: 2500 Asia 7963[2]	EU/US: 2500 Asia 7963[2]
Theoretical coverage of the paint	COVERAGE	[$m^2.l^{-1}$]		
Number of coats applied on the hull	Ncoats	[-]	2	2
Fraction excess paint applied[3]	Fexcess	[-]	0.20[4]	0.20
Fraction of the paint that is to be removed from the ships hull by HPW (exhausted paint)	Fwashing	[-]	0.20	0.20
Fraction of the paint that is to be removed from the ships hull by abrasion	Fabrasion	[-]	Reblasting[5]: 0.10	Spot blasting[5]: 0.005
Ratio reblasting/spot blasting[7]	$RATIO_{blasting}$	[-]	1/10	1/10
Fraction of a.i. remained in exhausted paint removed by HPW	$Fa.i._{exhpaint}$	[-]	0.05[1]	0.05[1]
Fraction of a.i. remained in old paint removed by abrasion	$Fa.i._{old\ paint}$	[-]	0.30[1]	0.30[1]
Fraction to surface water[8]	F_{water}	[-]	Max. 1	Max. 1
Fraction to soil	F_{soil}	[-]	0	0

1) Expert judgement CEPE.
2) Note that all other values are based on the European/US situation. Note also that the value for Asia is lower than for the new building scenario (Table 0.8) as also smaller ships are treated.
3) The theoretical paint demand is the amount of paint that is theoretically needed to paint the entire ship hull. The theoretical paint demand does not contain the excess paint applied on the hull due to overlap during the application process, the subsequent coating of join up seams and butts, etc. The theoretical paint demand and the excess paint together form the total amount of paint that is applied on the ships hull. This is important for the calculation of the amount of a.i. remained on the ships hull.
4) A fraction of 0.20 is the worst case value for the application of excess paint during M&R.
5) At reblasting the top layer of the old paint is removed from the entire ship hull, at spot blasting paint is removed only from parts of the hull.
6) Used for the calculation of the concentration during the emission period.
7) Expert judgement CEPE. Because spot blasting as well as reblasting occurs at the same shipyards, for the calculation of the yearly average concentration both spot blasting and reblasting has to be taken into account. Spot blasting removes paint from 5% of the hull area whereas reblasting removes paint from the total hull area (5% of 0.10 = 0.005).
8) Depending on the control measurements of the ship yard the emission up to a maximum of 100% either goes to surface water or to waste or a combination of these two.

Table III-172 Default settings for the calculation of the environmental concentrations for application and removal of the paint layer during M&R of commercial ships in an average OECD shipyard

Variable/parameter The removal frequency per year[1]	Unit [-]	Symbol Tfreq	Value 20[2]
Length of the harbour	[m]	LENGTHch	5000
Width of the harbour	[m]	WIDTHch	1000
Depth of the harbour	[m]	DEPTHch	15

III.3.6.15.4 Professional M&R pleasure craft

Application

Intermediate calculations:

$$Elocal_{soil} = \frac{\text{Vpaint} \cdot \text{Nboat} \cdot \text{F}_{\text{soil}} \cdot \text{Ca.i}}{\text{Tpaint}} \quad \textbf{(593)}$$

$$Elocal_{STP} = \frac{\text{Vpaint} \cdot \text{Nboat} \cdot \text{F}_{\text{STP}} \cdot \text{Ca.i}}{\text{Tpaint}} \quad \textbf{(594)}$$

Input

Tpaint	The painting period	[d]	D
Nboat	Number of boats treated per painting period	[-]	D
Vpaint	The theoretical amount of paint applied per boat	[l]	D
Ca.i.	The concentration of a.i. in the paint [g.l-1]	S	
F_{soil}	Fraction to soil	[-]	D
F_{STP}	Fraction to STP	[-]	D
Intermediate results			
Elocalsoil	Total emission to soil	[g.d-1]	O
ElocalSTP	Total emission to STP	[g.d-1]	O

Removal

Intermediate calculation:

$$Elocalsoil = \frac{(\text{Vpainttotal} \cdot \text{Nboat} \cdot \text{Ca.i} \cdot (\text{F}_{\text{washing}} \cdot \text{Fa.iexh paint} + \text{F}_{\text{abrasion}} \cdot \text{Fa.i oldpaint}) \cdot \text{F}_{\text{soil}})}{\text{Tremoval}} \quad \textbf{(595)}$$

$$ElocalSTP = \frac{(\text{Vpainttotal} \cdot \text{Nboat} \cdot \text{Ca.i} \cdot (\text{F}_{\text{washing}} \cdot \text{Fa.iexh paint} + \text{F}_{\text{abrasion}} \cdot \text{Fa.i oldpaint}) \cdot \text{F}_{\text{STP}})}{\text{Tremoval}} \quad \textbf{(596)}$$

$$Elocalwater = \frac{(\text{Vpainttotal} \cdot \text{Nboat} \cdot \text{Ca.i} \cdot (\text{F}_{\text{washing}} \cdot \text{Fa.iexh paint} + \text{F}_{\text{abrasion}} \cdot \text{Fa.i oldpaint}) \cdot \text{F}_{\text{water}})}{\text{Tremoval}} \quad \textbf{(597)}$$

Input			
Vpaint	The theoretical amount of paint applied per boat	[l]	D
Tremoval	The removal period	[d]	D
Nboat	Number of boats treated per removal period	[-]	D
Fwashing	Fraction of the paint that is to be removed from the ships hull by HPW (exhausted paint)	[-]	D
Fabrasion	Fraction of the paint that is to be removed from the ships hull by abrasion	[-]	D
Ca.i.	The concentration of active ingredient in the original paint	[g.l-1]	S
Fa.i.exhpaint	Fraction of a.i. remained in exhausted paint removed by HPW	[-]	D
Fa.i.old paint	Fraction of a.i. remained in old paint removed by abrasion	[-]	D
Fwater	Fraction to surface water	[-]	D
Fsoil	Fraction to soil	[-]	D
Intermediate results			
Elocalwater	Total emission to surface water	[g.d-1]	O
Elocalsoil	Total emission to soil	[g.d-1]	O
ElocalSTP	Total emission to STP	[g.d-1]	O

End calculation

Soil

See scenario for new building Pleasure craft (professional)

For the risk assessment the concentrations for application and removal has to be added.

STP

See scenario for new building Pleasure craft (professional)

For the risk assessment the concentrations in sludge for application and removal has to be added.
For water the highest concentration has to be used

Water

Harbour

$$\text{Clocalwater}_{\text{removal-1}} = \text{Elocalwater} / (\text{LENGTHch} * \text{WIDTHch} * \text{DEPTHch}) \qquad \textbf{(598)}$$

$$\text{Cwater}_{\text{removal/appl}} = \left(\text{Cwater}_{\text{removal/1 appl}} \cdot \frac{1 - \text{F}_{\text{rs}}^{183}}{1 - \text{F}_{\text{rs}}} \right) \qquad \textbf{(599)}$$

$$F_{rs} = e^{-k_{basin} \cdot T_{\text{interval}}} \qquad \textbf{(600)}$$

$$\boldsymbol{k_{advec,basin}} = \frac{\boldsymbol{ln\,2}}{\boldsymbol{DT50_{advec,basin}}} \qquad \textbf{(601)}$$

$$k_{basin} = \frac{kdeg_{water}}{1 + Kp_{susp.pest} \cdot SUSP_{water}} + k_{advec,basin} \qquad (602)$$

Input			
LENGTHch	Length of the harbour	[m]	D
WIDTHch	Width of the harbour	[m]	D
DEPTHch	Depth of the harbour	[m]	D
$F_{s\text{-}ns}$	fraction ships in yacht-basin	[-]	D
$Kp_{susp,pest}$	solids-water partition coefficient in suspended matter for pesticides	[$m^3.kg^{-1}$]	O
$SUSP_{water}$	concentration suspended matter	[$kg.m^{-3}$]	D
$kdeg_{water}$	degradation rate in surface water	[d^{-1}]	O
$DT50_{advec,basin}$	advection half-life time in basin	[d]	D
$k_{advec,basin}$	rate constant for advection	[d^{-1}]	O^c
k_{basin}	overall rate constant for removal from basin	[d^{-1}]	O^c
Tinterval	interval time for removal/application		
Output			
Clocalwater	peak concentration in water	[$kg_c.m^{-3}$]	O

River

See scenario for new building commercial ships

Table III-173 Default setting for the professional M&R of pleasure craft in an average OECD boat yard/marina: application of paint

Variable/parameter	**Symbol**	**Unit**	**Value for realistic worst case**	**Value for typical case**
The painting period	Tpaint	[d]	183[1] (6 months)	183[1] (6 months)
Number of boats treated per painting period	Nboat	[-]	50[2]	50[2]
The theoretical amount of paint applied per boat	Vpaint	[l]	4.5	4.5
Fraction to surface water	F_{water}	[-]	0	0
Fraction to STP[3]	F_{STP}	[-]	Max. 0.06	Max. 0.025
Fraction to soil[3]	F_{soil}	[-]	Max. 0.06[4]	Max. 0.025

1) Based on experience of representatives of industry in the OECD Steering Group on Anti-Fouling Products.
2) Based on 10% of the boats that are at berth in a realistic worst case marina (500). Approximately 10% of the boats are repaired professionally.
3) Depending on the control measurements of the boat yard the emission up to a maximum of 6% either goes to soil or a STP or a mixture between these two options.
4) Potential emission weighted for brush/roller and spray.

Table III-174 Default setting for the calculation of the environmental concentrations for professional application of paint during M&R of pleasure craft in an average OECD boat yard

Variable/parameter	Symbol	Unit	Value
The painting interval[1]	Tint	[month]	6
Length of the receiving soil compartment[2]	LENGTH	[m]	12.5
Width of the receiving soil compartment	WIDTH	[m]	5.5
Depth of the receiving soil compartment	DEPTH	[m]	0.1[3]
Soil density (dry weight)	$RHOsoil_{dw}$	[$kg.m^{-3}$]	1504[4]

1) Period in which painting does not occur.
2) A boat of 7.5 m length and 2.5 m width is assumed. For the determination of the surface of the receiving soil compartment a "walking path" around the boat for the applier of the paint is assumed. It was estimated that this path is 1 meter wide.
3) In line with the environmental emission scenario of the OECD for Wood Preservatives.
4) Based on EU-TGD (ECB, 2003) (wet weight is 1700 $kg.m^{-3}$).

Table III-175 Default setting for the professional removal of the paint layer in an average OECD boatyard

Variable/parameter	Symbol	Unit	Value for realistic worst case	Value for typical case
The removal period	Tremoval	[d]	183[1] (6 months)	183[1] (6 months)
Number of boats treated per removal period	Nboat	[-]	50[2]	50[2]
The amount of paint applied per boat	Vpaint	[l]	4.5 (as for application)	4.5 (as for application)
Fraction of the paint that is to be removed from the boat hull by HPW[3]	Fwashing	[-]	0.20	0.20
Fraction of the paint that is to be removed from the boat hull by abrasion[3]	Fabrasion	[-]	0.10	n/a
Fraction of a.i. remained in exhausted paint removed by washing[3]	$Fa.i._{\text{exh paint}}$	[-]	0.05	0.05
Fraction of a.i. remained in old paint removed by abrasion[3]	$Fa.i._{\text{old paint}}$	[-]	0.30	n/a
Fraction to surface water[4]	F_{water}	[-]	Max. 1	Max. 1
Fraction to STP[4]	F_{STP}	[-]	Max. 1	Max. 1
Fraction to soil[4]	F_{soil}	[-]	Max. 1	Max. 1

1) Based on expert judgement CEPE.
2) Based on 10% of the boats that are at berth in a realistic worst case marina (500). Approximately 10% of the boats are repaired professionally.
3) HP washing will remove only the leached layer. For pleasure boats the leached layer represents typically 20% of the paint film applied (Safinah, 2004) and contains a fraction of 0.05 (expert judgement CEPE) of the original concentration of of a.i. the paint. Abrasion will remove 30% of the old paint film. This 30% consists of the leached layer and an additional layer which contains a fraction of 0.30 (expert judgement CEPE) of the original concentration of of a.i. the paint (see also section **Error! Reference source not found.**).
4) Depending on the control measurements of the boatyard the emission goes to soil, surface water, or a STP or a mixture between these 3 options.

Table III-176 Default setting for the calculation of the local initial environmental concentrations in soil and surface water for professional application and removal of the paint layer during M&R of pleasure craft in an average OECD boatyard for both realistic worst and typical case

Variable/parameter	Unit	Symbol	Value
Soil			
The removal interval[1]	[month]	Tint	6
Length of the receiving soil compartment[2]	[m]	LENGTH	12.5
Width of the receiving soil compartment	[m]	WIDTH	5.5
Depth of the receiving soil compartment	[m]	DEPTH	0.1[3]
Soil density (dry weight)	$[kg.m^{-3}]$	$RHOsoil_{dw}$	1504[4]
Surface water			
Length	[m]	LENGTHm	141.5
Width	[m]	WIDTHm	141.5
Depth of harbour	[m]	DEPTHm	4
Advection time in basin (d^{-1})	$DT50_{advec,basin}$	[d]	50

1) Time period in which removal of paint does not occur.
2) The weighted average boat length of boats > 7.5 m is 10.36 m. A boat of 10.5 m length and 3.5 m width is assumed. For the determination of the surface of the receiving environmental compartment (compacted earth for the realistic worst case scenario) a “walking path” around the boat (width: 1 m) for the applier of the paint is assumed.
3) In line with the environmental emission scenario of the OECD for Wood Preservatives.
4) Based on EU-TGD (ECB, 2003) (wet weight is 1700 $kg.m^{-3}$).

III.3.6.15.5 Non-professional M&R pleasure craft

Application

Intermediate calculations:

$$\mathrm{E}\mathit{local}_{soil} = \mathrm{Vpaint} \cdot \mathrm{F}_{\mathrm{soil}} \cdot \mathrm{Ca.i} - \qquad \textbf{(603)}$$

$$\mathrm{E}\mathit{local}_{STP} = \mathrm{Vpaint} \cdot \mathrm{F}_{\mathrm{STP}} \cdot \mathrm{Ca.i} \qquad \textbf{(604)}$$

Input			
Vpaint	The theoretical amount of paint applied per boat	[l]	D
Ca.i.	The concentration of a.i. in the paint [g.l-1]	S	
F_{soil}	Fraction to soil	[-]	D
F_{STP}	Fraction to STP	[-]	D

Intermediate results			
Elocalsoil	Total emission to soil	[g.d-1]	O
ElocalSTP	Total emission to STP	[g.d-1]	O

Note: for this scenario it is assumed that 5 boats will be painted during 5 days. In EUSES this is indicated as number of applications. For the calculation of the total emission on a daily base the number of boats is not relevant

Removal

In this scenario an extra parameter (Ndays) is used to express the fact that during a time period of 3 months it takes 5 days to treat 5 boats. The remaining 9 months of the year removal does not occur.

Intermediate calculation:

$$\mathrm{E}\mathit{localsoil} = \frac{(\mathrm{Vpainttotal} \cdot \mathrm{Nboat} \cdot \mathrm{Ca.i} \cdot (\mathrm{F}_{\mathrm{washing}} \cdot \mathrm{Fa.iexh\,paint} + \mathrm{F}_{\mathrm{abrasion}} \cdot \mathrm{Fa.i\,oldpaint}) \cdot \mathrm{F}_{\mathrm{soil}})}{\mathrm{Tremoval}} \qquad \textbf{(605)}$$

$$\mathrm{E}\mathit{localSTP} = \frac{(\mathrm{Vpainttotal} \cdot \mathrm{Nboat} \cdot \mathrm{Ca.i} \cdot (\mathrm{F}_{\mathrm{washing}} \cdot \mathrm{Fa.iexh\,paint} + \mathrm{F}_{\mathrm{abrasion}} \cdot \mathrm{Fa.i\,oldpaint}) \cdot \mathrm{F}_{\mathrm{STP}})}{\mathrm{Tremoval}} \qquad \textbf{(606)}$$

$$\mathrm{E}\mathit{localwater} = \frac{(\mathrm{Vpainttotal} \cdot \mathrm{Nboat} \cdot \mathrm{Ca.i} \cdot (\mathrm{F}_{\mathrm{washing}} \cdot \mathrm{Fa.iexh\,paint} + \mathrm{F}_{\mathrm{abrasion}} \cdot \mathrm{Fa.i\,oldpaint}) \cdot \mathrm{F}_{\mathrm{water}})}{\mathrm{Tremoval}} \qquad \textbf{(607)}$$

Input			
Vpaint	The theoretical amount of paint applied per boat	[l]	D
Tremoval	The removal period	[d]	D
Nboat	Number of boats treated per removal period	[-]	D
Fwashing	Fraction of the paint that is to be removed from the ships hull by HPW (exhausted paint)	[-]	D
Fabrasion	Fraction of the paint that is to be removed from the ships hull by abrasion	[-]	D
Ca.i.	The concentration of active ingredient in the original paint	[g.l-1]	S
Fa.i.exhpaint	Fraction of a.i. remained in exhausted paint removed by HPW	[-]	D
Fa.i.old paint	Fraction of a.i. remained in old paint removed by abrasion	[-]	D
Fwater	Fraction to surface water	[-]	D
Fsoil	Fraction to soil	[-]	D
Intermediate results			
Elocalwater	Total emission to surface water	[g.d-1]	O
Elocalsoil	Total emission to soil	[g.d-1]	O
ElocalSTP	Total emission to STP	[g.d-1]	O

End calculation

Soil

See scenario for new building Pleasure craft (professional)

For the risk assessment the concentrations for application and removal has to be added.

STP

See scenario for new building Pleasure craft (professional)

For the typical case the concentration in sludge is divided by 18.2 (=91/5) to calculate an average concentration. For the worst case this is not necessary (daily emission)

For the risk assessment the concentrations in sludge for application and removal has to be added.
For water the highest concentration has to be used.

Water

Harbour

$$Clocalwater_{removal\text{-}1} = Elocalwater \,/\, (LENGTHch * WIDTHch * DEPTHch) \qquad \textbf{(608)}$$

Realistic worst case

$$Cwater_{removal} = \left(Cwater_{removal\text{-}1\,appl} \cdot \frac{1 - F_{rs}^{91}}{1 - F_{rs}} \right) \qquad \textbf{(609)}$$

$$F_{rs} = e^{-k_{basin} \cdot T_{interval}}$$

$$k_{advec,basin} = \frac{ln\,2}{DT50_{advec,basin}} \qquad (610)$$

$$k_{basin} = \frac{kdeg_{water}}{1 + Kp_{susp.pest} \cdot SUSP_{water}} + k_{advec,basin} \qquad (611)$$

Input			
LENGTHch	Length of the harbour	[m]	D
WIDTHch	Width of the harbour	[m]	D
DEPTHch	Depth of the harbour	[m]	D
$F_{s\text{-}ns}$	fraction ships in yacht-basin	[-]	D
$Kp_{susp,pest}$	solids-water partition coefficient in suspended matter for pesticides	[$m^3.kg^{-1}$]	O
$SUSP_{water}$	concentration suspended matter	[$kg.m^{-3}$]	D
$kdeg_{water}$	degradation rate in surface water	[d^{-1}]	O
$DT50_{advec,basin}$	advection half-life time in basin	[d]	D
$k_{advec,basin}$	rate constant for advection	[d^{-1}]	O^c
k_{basin}	overall rate constant for removal from basin	[d^{-1}]	O^c
Output			
Clocalwater	peak concentration in water	[$kg_c.m^{-3}$]	O

River

See scenario for new building commercial ships

Table III-177 Default setting for the non-professional M&R of pleasure craft in an average OECD marina: application of paint

Variable/parameter	**Unit**	**Symbol**	**Value**
The painting period	[d]	Tpaint	91[1] (3 months)
Number of days to paint one boat[2]	[-]	Ndays	1
Number of boats treated per painting period	[-]	Nboat	5[3]
The theoretical amount of paint applied per boat	[l]	Vpaint	2.5[1]
Fraction to surface water	[-]	F_{water}	0
Fraction to STP[4]	[-]	F_{STP}	Max. 0.025
Fraction to soil[4]	[-]	F_{soil}	Max. 0.025

1) Expert judgement CEPE.

2) In this scenario an extra parameter (Ndays) is used to express the fact that during a time period of 3 months it takes 5 days to paint 5 boats. The remaining 9 months of the year painting does not occur.

3) 10% of the boats are repaired professionally (Safinah) and that 20% of the boats are not painted at all per year (expert judgement industry). Thus 350 (70%) of the boats that are at berth in a realistic worst case marina (500) are repaired non-professionally each year. During 3 months 350 boats are painted. This does not necessarily happen at the same spot of 9.5 m length and 4.5 m width (boats can be taken home for application or painted in storage area). Therefore it is assumed that only 5 boats are painted on the same spot per painting period (based on Finnish data: In Finland typically 1-5 boats are painted on the same spot).

4) Depending on the control measurements (hard standing area) the emission up to a maximum of 2.5% either goes to soil or a STP or a mixture between these two options. For non-professional application it is most likely that the emission goes to soil.

Table III-178 Default setting for the calculation of the environmental concentrations for non-professional application of paint during M&R of pleasure craft in an average OECD marina for both realistic worst case and typical case scenario

Variable/parameter	**Unit**	**Symbol**	**Value**	**S/D/O/P**
The painting interval[1]	[month]	Tint	9	D
Length of the receiving soil compartment[2]	[m]	LENGTH	9.5	D
Width of the receiving soil compartment	[m]	WIDTH	4.5	D
Depth of the receiving soil compartment	[m]	DEPTH	0.1[3]	D
Soil density (dry weight)	$[kg.m^{-3}]$	$RHOsoil_{dw}$	1504[4]	

1) Period in which painting does not occur.
2) A boat of 7.5 m length and 2.5 m width is assumed. For the determination of the surface of the receiving soil compartment a "walking path" around the boat for the applier of the paint is assumed. It was estimated that this path is 1 metre wide.
3) In line with the environmental emission scenario of the OECD for Wood Preservatives.
4) Based on EU-TGD (ECB, 2003) (wet weight is 1700 $kg.m^{-3}$).

Table III-179 Default setting for the Non-professional removal of the paint layer in an average OECD boatyard/marina

Variable/parameter	**Symbol**	**Unit**	**Value for realistic worst case**	**Value for typical case**
The removal period	Tremoval	[d]	91[1] (3 months)	91[1] (3 months)
The number of days for the treatment of one boat[5]	Ndays	[-]	n/a	1
Number of boats treated per removal period	Nboat	[-]	350[2]	5
The amount of paint applied per boat	Vpaint	[l]	2.5	2.5
Fraction of the paint that is to be removed from the boat hull by HPW[3]	Fwashing	[-]	0.20	n/a
Fraction of the paint that is to be removed from the boat hull by abrasion[3]	Fabrasion	[-]	n/a	0.10
Fraction of a.i. remained in exhausted paint removed by washing[3]	$Fa.i._{exh\ paint}$	[-]	0.05	n/a
Fraction of a.i. remained in old paint removed by abrasion[3]	$Fa.i._{old\ paint}$	[-]	n/a	0.30
Fraction to surface water[4]	F_{water}	[-]	Max. 1	n/a
Fraction to STP[4]	F_{STP}	[-]	Max. 1	Max. 1
Fraction to soil[4]	F_{soil}	[-]	Max. 1	Max. 1

1) Based on expert judgement of CEPE.
2) Based on the fact that 10% of the boats are repaired professionally (Safinah 2004) and that 20% of the boats are not painted at all per year (expert judgement industry). Thus 70% of the boats that are at berth in a realistic worst case marina (500) are repaired non-professionally each year.
3) HP washing will remove only the leached layer. For pleasure boats the leached layer represents typically 20% of the paint film applied (Safinah, 2004) and contains a fraction of 0.05 (expert judgement CEPE) of the original concentration of of a.i. the paint. Abrasion will remove 30% of the old paint film. This 30% consists of the leached layer and an additional layer which contains a fraction of 0.30 (expert judgement CEPE) of the original concentration of of a.i. the paint.
4) Depending on the control measurements of the boatyard the emission goes to soil, surface water or a STP or a mixture between these 3 options.
5) In this scenario an extra parameter (Ndays) is used to express the fact that during a time period of 3 months it takes 5 days to treat 5 boats. The remaining 9 months of the year removal does not occur.

Table III-180 Default setting for calculation of the environmental concentrations in soil and surface water for non-professional removal of the paint layer in an average OECD boatyard/marina (see M&R) for both realistic worst and typical case

Variable/parameter *Soil*	**Symbol**	**Unit**	**Value**
The removal interval[1)]	Tint	[month^{-1}]	9
The removal frequency	Tfreq	[-]	5
Length of the receiving soil compartment[2)]	LENGTH	[m]	9.5
Width of the receiving soil compartment	WIDTH	[m]	4.5
Depth of the receiving soil compartment	DEPTH	[m]	0.1[3)]
Soil density (dry weight)	$RHOsoil_{dw}$	[kg.m^{-3}]	1504[4)]
Surface water			
Length	LENGTHm	[m]	141.5
Width	WIDTHm	[m]	141.5
Depth of harbour	DEPTHm	[m]	4
Advection time in basin (d^{-1})	$DT50_{advec,basin}$	[d]	50

1) Time period in which removal of paint does not occur.

2) A boat of 7.5 m length and 2.5 m width is assumed. For the determination of the surface of the receiving soil compartment a “walking path” around the boat for the applier of the paint is assumed. It was estimated that this path is 1 metre wide.

3) In line with the environmental emission scenario of the OECD for Wood Preservatives.

4) Based on EU-TGD (ECB, 2003) (wet weight is 1700 kg.m^{-3}).

III.3.6.16 Embalming and taxidermist fluids

The scenarios and models and calculation formulations used in this version of EUSES 2.1.1 for insecticides have been taken from the following document:

- European Union System for the Evaluation of Substances, EUSES 2.0 (EC, 2004)

Taxidermy includes the preservation of animals and concerns as well as large mammals, fishes, birds and reptiles. Embalming consist of three different procedures which involve the use of biocides: surface disinfection (soaps, solutions), arterial injection of fluids and injection of cavity fluids into the torso to substitute body fluids.

III.3.6.16.1 Biocides used in taxidermy

Model for calculating release to water for compounds used in taxidermist fluids.

$$Elocal\_water_i = Qskin \cdot Qsubst \cdot (1 - Ffix) \qquad (612)$$

$$Elocal_{water} = \sum Elocal\_water_i \qquad (613)$$

Input			
Qskin	quantity of treated drained skin per day	[kg.d^{-1}]	D
-	type of agent per treatment step	[-]	P
Qsubst	quantity of active substance applied per kg of drained skin	[kg.kg^{-1}]	O
Ffix	fixation fraction	[-]	S/D
$Elocal\_water_i$	local emission of active substance to waste water for treatment step *i*	[kg.d^{-1}]	O
Output			
$Elocal_{water}$	local emission of active substance to waste water for all treatment steps	[kg$_c$.d^{-1}]	O

Table III-181 Default settings of the model for calculating the release of biocides used in taxidermy.

Parameter	**Symbol**	**Unit**	**Value**
Quantity of treated drained skin per day	Qskin	[kg.d^{-1}]	4
Quantity of active substance applied per kg of drained skin Pickling - formaldehyde - tanning agent Soaking - bactericide Preservation - insecticide	Qsubst	[kg.kg^{-1}]	0.02 0.005 0.02 0.002 0.02
Fixation fraction	Ffix	[-]	0.95

III.3.6.16.2 Biocides used in the embalming process

Model for calculating release to water for compounds used in the embalming process.

$$\begin{aligned} Elocal_{water} = & Vform_{arterial} \cdot RHOform \cdot Cform_{arterial} \cdot (1 - Fret_{arterial}) + \\ & Vform_{cavity} \cdot RHOform \cdot Cform_{cavity} \cdot (1 - Fret_{cavity}) \end{aligned} \tag{614}$$

Input			
-	type of preservation and type of biocide applied	[-]	P
$Vform_{arterial}$	volume of solution applied per embalmed corpse for arterial injection	[m^3]	O
$Vform_{cavity}$	volume of solution applied per embalmed corpse for cavity treatment	[m^3]	O
RHOform	specific mass of solution	[$kg.m^{-3}$]	D
$Cform_{arterial}$	content of active substance in solution for arterial injection	[$kg.kg^{-1}$]	S
$Cform_{cavity}$	content of active substance in solution for cavity treatment	[$kg.kg^{-1}$]	S
$Fret_{arterial}$	retention rate of arterial fluid	[-]	S/O
$Fret_{cavity}$	retention rate of cavity fluid	[-]	S/O
Output			
$Elocal_{water}$	local emission of active substance to waste water	[$kg.d^{-1}$]	O

Table III-182 Default settings of the model for calculating the release of biocides used in the embalming process.

Parameter	**Symbol**	**Unit**	**Value**
Volume of solution applied per embalmed corpse for both arterial injection and cavity treatment	$Vform_{arterial}$ / $Vform_{cavity}$	[m^3]	
Short-term			
- formaldehyde 4%			0.0060
- formaldehyde 22%			0.0005
Long-term			
- formaldehyde 4%			0.0100
- formaldehyde 22%			0.0005
Retention rate of both arterial injection fluid and cavity treatment fluid	$Fret_{arterial}$ / $Fret_{cavity}$	[-]	
Short-term			
- formaldehyde 4%			0.9
- formaldehyde 22%			0.9
Long-term			
- formaldehyde 4%			0.8
- formaldehyde 22%			0.9
Specific mass of solution	RHOform	[$kg.m^{-3}$]	1,000

III.3.6.16.3 Biocides releases in cemeteries

Model for calculating release in cemeteries of compounds used in the embalming process.

$$\begin{aligned} Elocal_{soil} = {} & [Vform_{arterial} \cdot RHOform \cdot Cform_{arterial} \cdot (1 - Fret_{arterial}) \\ & + Vform_{cavity} \cdot RHOform \cdot Cform_{cavity} \cdot (1 - Fret_{cavity})] \cdot \\ & (1 - Freact) \cdot Ncorpse \end{aligned} \qquad (615)$$

$$\begin{aligned} Csoil\_av_{cem} = {} & Elocal_{soil} \; / \; (LENGTHcem \cdot WIDTHcem \cdot DEPTHmix_{cem-soil} \\ & \cdot RHOsoil \cdot krem_{soil}) \end{aligned} \qquad (616)$$

$$Cporew\_av_{cem} = Csoil\_av_{cem} \cdot RHOsoil \; / \; K_{soil-water} \qquad (617)$$

Input			
-	type of preservation and type of biocide applied	[-]	P
$Vform_{arterial}$	volume of solution applied per embalmed corpse for arterial injection	[m^3]	O
$Vform_{cavity}$	volume of solution applied per embalmed corpse for cavity treatment	[m^3]	O
RHOform	specific mass of solution	[$kg.m^{-3}$]	D
$Cform_{arterial}$	content of active substance in solution for arterial injection	[$kg.kg^{-1}$]	S
$Cform_{cavity}$	content of active substance in solution for cavity treatment	[$kg.kg^{-1}$]	S
$Fret_{arterial}$	retention rate of arterial fluid	[-]	S/O
$Fret_{cavity}$	retention rate of cavity fluid	[-]	S/O
Freact	factor for reaction with body	[-]	S/D
Ncorpse	number of embalmed corpses buried per day	[-]	D
LENGTHcem	length of cemetery	[m]	D
WIDTHcem	width of cemetery	[m]	D
$DEPTHmix_{cem-soil}$	mixing depth of soil	[m]	D
RHOsoil	bulk density of soil	[$kg.m^{-3}$]	D
$K_{soil-water}$	soil-water partition coefficient	[$m^3.m^{-3}$]	O^c
$krem_{soil}$	first order rate constant for removal in soil	[d^{-1}]	O
$Elocal_{soil}$	daily average input of active substance to the cemetery	[$kg.d^{-1}$]	O
$Csoil\_av_{cem}$	average concentration in soil	[$kg.kg_{wwt}^{-1}$]	O
Output			
$Cporew\_av_{cem}$	average concentration in soil pore water	[$kg.m^{-3}$]	O

Table III-183 Default settings of the model for calculating the release in cemeteries of biocides used in the embalming process.

Parameter	**Symbol**	**Unit**	**Value**
Volume of solution applied per embalmed corpse for both arterial injection and cavity treatment	$Vform_{arterial}$ / $Vform_{cavity}$	[m^3]	
Short-term			
- formaldehyde 4%			0.0060
- formaldehyde 22%			0.0005
Long-term			
- formaldehyde 4%			0.0100
- formaldehyde 22%			0.0005
Retention rate of both arterial injection fluid and cavity treatment fluid	$Fret_{arterial}$ / $Fret_{cavity}$	[-]	
Short-term			
- formaldehyde 4%			0.9
- formaldehyde 22%			0.9
Long-term			
- formaldehyde 4%			0.8
- formaldehyde 22%			0.9
Specific mass of solution	RHOform	[$kg.m^{-3}$]	1,000
Factor for reaction with body	Freact	[-]	0
Daily number of embalmed corpses buried per day	Ncorpse	[-]	0.065
Length of cemetery	LENGTHcem	[m]	100
Width of cemetery	WIDTHcem	[m]	100
Mixing depth of soil	$DEPTHmix_{cem-soil}$	[m]	0.5
Bulk density of soil	RHOsoil	[$kg.m^{-3}$]	1,700
Specific mass of solution	RHOform	[$kg.m^{-3}$]	1,000

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III.4 ENVIRONMENTAL DISTRIBUTION

In the environmental distribution module, five sub-modules are specified:
- Estimation of partition coefficients.
- Estimation of environmental degradation rates.
- Fate in sewage treatment.
- Regional environmental distribution.
- Local environmental distribution.

Environmental distribution is estimated on three spatial scales: local, regional and continental. The environmental characteristics of these scales are (by default) the same.

III.4.1 Partition coefficients

In this section, the characteristics of the environmental compartments are defined. From this definition, the bulk densities of soil, sediment and suspended matter are calculated. The following partitioning processes are quantified in this section:
- Adsorption to aerosol particles.
- Air-water partitioning.
- Adsorption/desorption to solids in soil, sediment, suspended matter and sewage sludge.

The output parameters for bulk densities of compartments and 'dimensionless partition coefficients' are closed for the user. This is done for the sake of internal consistency. For example bulk density of soil is defined by the fractions and densities of the separate phases (solids, water, air). The bulk density should not be changed without changing the fractions or densities of the phases.

Input			
VP	vapour pressure	[Pa]	
MOLW	molecular weight	$[kg_c.mol^{-1}]$	
SOL	solubility	$[kg_c.m^{-3}]$	
Kow	octanol-water partition coefficient	[-]	
TEMPmelt	melting point (only for solids for estimating $Fass_{aer}$)	[K]	
Intermediate results			
VP_L	sub-cooled liquid vapour pressure	[Pa]	
Koc	organic carbon-water partition coefficient	$[m^3.kg^{-1}]$	
Output 1			
RHO_{soil}	wet bulk density of soil	$[kg_{wwt}.m^{-3}]$	c
RHO_{sed}	wet bulk density of sediment	$[kg_{wwt}.m^{-3}]$	c
RHO_{susp}	wet bulk density of suspended matter	$[kg_{wwt}.m^{-3}]$	c
$CONV_{soil}$	conversion factor for soil concentrations: wwt to dwt	$[kg_{wwt}.kg_{dwt}^{-1}]$	c
$CONV_{sed}$	conversion factor for sediment concentrations: wwt to dwt	$[kg_{wwt}.kg_{dwt}^{-1}]$	c
$Fass_{aer}$	fraction of chemical associated with aerosol particles	[-]	
HENRY	Henry's law constant	$[Pa.m^3.mol^{-1}]$	
Kp_{susp}	solids-water partition coefficient in suspended matter	$[m^3.kg^{-1}]$	
Kp_{sed}	solids-water partition coefficient in sediment	$[m^3.kg^{-1}]$	
Kp_{soil}	solids-water partition coefficient in soil	$[m^3.kg^{-1}]$	
Kp_{RS}	solids-water partition coeff. in raw sewage sludge	$[m^3.kg^{-1}]$	
Kp_{PS}	solids-water partition coeff. in settled sewage sludge	$[m^3.kg^{-1}]$	
Kp_A	solids-water partition coeff. in activated sewage sludge	$[m^3.kg^{-1}]$	
Kp_{SLS}	solids-water partition coeff. in effluent sewage sludge	$[m^3.kg^{-1}]$	
Output 2 (internal parameters)			
$K_{air-water}$	air-water partition coefficient	$[m^3.m^{-3}]$	c
$K_{soil-water}$	soil-water partition coefficient	$[m^3.m^{-3}]$	c
$K_{susp-water}$	suspended matter-water partition coefficient	$[m^3.m^{-3}]$	c
$K_{sed-water}$	sediment-water partition coefficient	$[m^3.m^{-3}]$	c

Table III-184 *Default environmental characteristics for local, regional and continental scales*

Parameter	**Symbol**	**Unit**	**Value**
General			
Density of solid phase	RHOsolid	$[kg_{solid}.m_{solid}^{-3}]$	2500
Density of water phase	RHOwater	$[kg_{water}.m_{water}^{-3}]$	1000
Density of air	RHOair	$[kg_{air}.m_{air}^{-3}]$	1.3
Environmental temperature Freshwater environment (12 °C) Marine environment (12 °C)	TEMP	[K]	 285 285 [c]
Constant of Junge equation	CONjunge	[Pa.m]	[a]
Specific surface area of aerosol particles	$SURF_{aer}$	$[m^2.m^{-3}]$	[a]
Gas constant	R	$[Pa.m^3.mol^{-1}.K^{-1}]$	8.314 [b]
Suspended matter			
Volume fraction of solids in susp. matter	$Fsolid_{susp}$	$[m_{solid}^3.m_{susp}^{-3}]$	0.1
Volume fraction of water in susp. matter	$Fwater_{susp}$	$[m_{water}^3.m_{susp}^{-3}]$	0.9
Weight fraction of organic carbon in susp. solids	Foc_{susp}	$[kg_{oc}.kg_{solid}^{-1}]$	0.1
Sediment			
Volume fraction of solids in sediment	$Fsolid_{sed}$	$[m_{solid}^3.m_{sed}^{-3}]$	0.2
Volume fraction of water in sediment	$Fwater_{sed}$	$[m_{water}^3.m_{sed}^{-3}]$	0.8
Weight fraction of organic carbon sediment solids	Foc_{sed}	$[kg_{oc}.kg_{solid}^{-1}]$	0.05
Soil			
Volume fraction of solids in soil	$Fsolid_{soil}$	$[m_{solid}^3.m_{soil}^{-3}]$	0.6
Volume fraction of water in soil	$Fwater_{soil}$	$[m_{water}^3.m_{soil}^{-3}]$	0.2
Volume fraction of air in soil	$Fair_{soil}$	$[m_{air}^3.m_{soil}^{-3}]$	0.2
Weight fraction of organic carbon in soil solids	Foc_{soil}	$[kg_{oc}.kg_{solid}^{-1}]$	0.02

[a] By default, the product of *CONjunge* and *SURF*$_{aer}$ is set to 10^{-4} Pa (Van de Meent, 1993); Den Hollander and Van de Meent (2004) uses $2.58.10^{-5}$ Pa.

[b] This default cannot be changed by the user.

[c] Although the TGD (2003) proposed a temperature of 9 °C, due to the small differences it was decided to keep the temperature the same for all compartments on the moderate global scale the same.

III.4.1.1 Bulk densities of compartments

Each of the compartments soil, sediment, and suspended matter is described as consisting of three phases: air (relevant in soil only), solids and water. The bulk density of each compartment is thus defined by the fraction and bulk density of each phase. Both the fractions of solids and water, and the total bulk density are used in subsequent calculations. This implies that the bulk density of a compartment cannot be changed independently of the fractions of the separate phases and vice versa.

$$RHO_{soil} = Fsolid_{soil} \cdot RHOsolid + Fwater_{soil} \cdot RHOwater + Fair_{soil} \cdot RHOair \qquad (618)$$

$$RHO_{sed} = Fsolid_{sed} \cdot RHOsolid + Fwater_{sed} \cdot RHOwater \qquad (619)$$

$$RHO_{susp} = Fsolid_{susp} \cdot RHOsolid + Fwater_{susp} \cdot RHOwater \qquad (620)$$

Input			
$Fwater_{soil}$	volume fraction of water in soil	$[m^3.m^{-3}]$	D
$Fsolid_{soil}$	volume fraction of solids in soil	$[m^3.m^{-3}]$	D
$Fair_{soil}$	volume fraction of air in soil	$[m^3.m^{-3}]$	D
$Fwater_{sed}$	volume fraction of water in sediment	$[m^3.m^{-3}]$	D
$Fsolid_{sed}$	volume fraction of solids in sediment	$[m^3.m^{-3}]$	D
$Fwater_{susp}$	volume fraction of water in suspended matter	$[m^3.m^{-3}]$	D
$Fsolid_{susp}$	volume fraction of solids in suspended matter	$[m^3.m^{-3}]$	D
RHOsolid	density of solid phase	$[kg.m^{-3}]$	D
RHOwater	density of water phase	$[kg.m^{-3}]$	D
RHOair	density of air phase	$[kg.m^{-3}]$	D
Output			
RHO_{soil}	wet bulk density of soil	$[kg_{wwt}.m^{-3}]$	O^c
RHO_{sed}	wet bulk density of sediment	$[kg_{wwt}.m^{-3}]$	O^c
RHO_{susp}	wet bulk density of suspended matter	$[kg_{wwt}.m^{-3}]$	O^c

III.4.1.2 Conversion wet weight-dry weight

In EUSES, concentrations in soil and sediment are total concentrations, and therefore expressed on a wet-weight basis. Optionally, intermediate results can be presented and changed on dry-weight basis. The conversion factors for soil and sediment are derived from the compartment definition in phases. The conversion to dry weight can also be used for entering terrestrial toxicity data.

$$CONV_{soil} = \frac{RHO_{soil}}{Fsolid_{soil} \cdot RHOsolid} \qquad (621)$$

$$CONV_{susp} = \frac{RHO_{susp}}{Fsolid_{susp} \cdot RHOsolid} \qquad (622)$$

Input			
RHO_{soil}	wet bulk density of soil	$[kg_{wwt}.m^{-3}]$	O^c
$Fsolid_{soil}$	volume fraction of solids in soil	$[m^3.m^{-3}]$	D
RHO_{susp}	wet bulk density of suspended matter	$[kg_{wwt}.m^{-3}]$	O^c
$Fsolid_{susp}$	volume fraction of solids in suspended matter	$[m^3.m^{-3}]$	D
RHOsolid	density of solid phase	$[kg.m^{-3}]$	D
Output			
$CONV_{soil}$	conversion factor for soil concentrations: wwt to dwt	$[kg_{wwt}.kg_{dwt}^{-1}]$	O^c
$CONV_{susp}$	conversion factor for suspended matter conc.: wwt to dwt	$[kg_{wwt}.kg_{dwt}^{-1}]$	O^c

III.4.1.3 Adsorption to aerosol particles

The fraction of the chemical associated with aerosol particles can be estimated on the basis of the chemical's vapour pressure, according to Junge (1977). In this equation, the sub-cooled liquid vapour pressure should be used. For solids, a correction is applied according to Mackay (1991).

$$Fass_{aer} = \frac{CONjunge \cdot SURF_{aer}}{VP_L + CONjunge \cdot SURF_{aer}} \qquad \textbf{(623)}$$

If *TEMPmelt* <= *TEMP* (substance is liquid):

$$VP_L = VP \qquad \textbf{(624)}$$

If *TEMPmelt* > *TEMP* (substance is solid):

$$VP_L = \frac{VP}{e^{6.79\left(1 - \frac{TEMPmelt}{TEMP}\right)}} \qquad \textbf{(625)}$$

Input			
CONjunge	constant of Junge equation	[Pa.m]	D
$SURF_{aer}$	surface area of aerosol particles	$[m^2.m^{-3}]$	D
VP	vapour pressure	[Pa]	S
TEMP	environmental temperature	[K]	D
TEMPmelt	melting point of substance	[K]	S
Output			
VP_L	sub-cooled liquid vapour pressure	[Pa]	O
$Fass_{aer}$	fraction of chemical associated with aerosol particles	[-]	O

III.4.1.4 Air-water partitioning

The transfer of substances from the aqueous phase to the gas phase (e.g. stripping in the aeration tank of an STP, volatilisation from surface water) is estimated by means of its Henry's Law constant. If the value is not available in the input dataset, the required Henry's Law constant and $K_{air\text{-}water}$ (also known as the 'dimensionless' Henry's Law constant) can be estimated from the ratio of the vapour pressure to the water solubility:

$$HENRY = \frac{VP \cdot MOLW}{SOL} \qquad \textbf{(626)}$$

$$K_{air\text{-}water} = \frac{HENRY}{R \cdot TEMP} \qquad \textbf{(627)}$$

Input			
VP	vapour pressure	[Pa]	S
MOLW	molecular weight	[$kg_c.mol^{-1}$]	S
SOL	water solubility	[$kg_c.m^{-3}$]	S
R	gas constant	[$Pa.m^3.mol^{-1}.K^{-1}$]	D^c
TEMP	environmental temperature	[K]	D
Output			
HENRY	Henry's law constant	[$Pa.m^3.mol^{-1}$]	O
$K_{air\text{-}water}$	air-water partition coefficient	[$m^3.m^{-3}$]	O^c

III.4.1.5 Estimation of Koc

If no *Koc* is available from the dataset, it may be estimated from *Kow*. Several models have been developed for different classes of chemicals. Most relationships are based on *Kow*, since hydrophobic interactions are the most dominant type of interactions between non-polar organic chemicals and the soil organic carbon. Chapter 4 of the TGD discusses these estimation routines in more detail, and proposes the following general defaulte for non-polar, organic compounds (Sabljic *et al.*, 1995). The QSAR was derived from a range of log *Kow* values from 1 - 7.5. For specific groups of substances, other QSARs are available, which are presented in Table III-185. Euses will present these formulas to the user. These QSARs should be used, if appropriate, and the estimate of equation **(628)** will be overwritten in such cases (Sabljic *et al.*, 1995).

$$Koc = \frac{1.26 \cdot Kow^{0.81}}{1000} \qquad \textbf{(628)}$$

Input			
Kow	octanol-water partition coefficient	[-]	S
Output			
Koc	organic carbon-water partition coefficient:	[$m^3.kg^{-1}$]	O

Table III-185 *QSARS for soil and sediment sorption for different chemical classes (Sabljic et al, 1995).*

Chemical class	**Equation**
Predominantly hydrophobics	$Koc = \frac{1.26 \cdot Kow^{0.81}}{1000}$
Nonhydrophobics	$Koc = \frac{10.47 \cdot Kow^{0.52}}{1000}$
Phenols, anilines, benzonitriles, nitrobenzenes	$Koc = \frac{7.94 \cdot Kow^{0.63}}{1000}$
Acetanilides, carbamates, esters, phenylureas, phosphates, triazines, triazoles, uracils	$Koc = \frac{12.30 \cdot Kow^{0.47}}{1000}$
Alcohols, organic acids	$Koc = \frac{3.16 \cdot Kow^{0.47}}{1000}$
Acetanilides	$Koc = \frac{13.18 \cdot Kow^{0.40}}{1000}$
Alcohols	$Koc = \frac{3.16 \cdot Kow^{0.39}}{1000}$
Amides	$Koc = \frac{17.78 \cdot Kow^{0.33}}{1000}$
Anilines	$Koc = \frac{7.08 \cdot Kow^{0.62}}{1000}$
Carbamates	$Koc = \frac{13.80 \cdot Kow^{0.37}}{1000}$
Dinitroanilines	$Koc = \frac{83.18 \cdot Kow^{0.38}}{1000}$
Esters	$Koc = \frac{11.22 \cdot Kow^{0.49}}{1000}$
Nitrobenzenes	$Koc = \frac{3.55 \cdot Kow^{0.77}}{1000}$
Organic acids	$Koc = \frac{2.09 \cdot Kow^{0.60}}{1000}$
Phenols, benzonitriles	$Koc = \frac{12.02 \cdot Kow^{0.57}}{1000}$
Phenylureas	$Koc = \frac{11.22 \cdot Kow^{0.49}}{1000}$
Phosphates	$Koc = \frac{14.79 \cdot Kow^{0.49}}{1000}$
Triazines	$Koc = \frac{31.62 \cdot Kow^{0.30}}{1000}$
Triazoles	$Koc = \frac{25.70 \cdot Kow^{0.47}}{1000}$

III.4.1.6 Solids-water partitioning in the environment

The solids-water partition coefficient (*Kp*) in each environmental compartment (soil, sediment, suspended matter) can be derived from the normalised partition coefficient, *Koc*, and the fraction of organic carbon in the compartment.

$$Kp_{soil} = Foc_{soil} \cdot Koc \tag{629}$$

$$Kp_{sed} = Foc_{sed} \cdot Koc \tag{630}$$

$$Kp_{susp} = Foc_{susp} \cdot Koc \tag{631}$$

Input			
Foc_{soil}	weight fraction of organic carbon in soil	$[kg.kg^{-1}]$	D
Foc_{sed}	weight fraction of organic carbon in sediment	$[kg.kg^{-1}]$	D
Foc_{susp}	weight fraction of organic carbon in suspended matter	$[kg.kg^{-1}]$	D
Koc	organic carbon-water partition coefficient	$[m^3.kg^{-1}]$	O
Output			
Kp_{susp}	solids-water partition coefficient in suspended matter	$[m^3.kg^{-1}]$	O
Kp_{sed}	solids-water partition coefficient in sediment	$[m^3.kg^{-1}]$	O
Kp_{soil}	solids-water partition coefficient in soil	$[m^3.kg^{-1}]$	O

III.4.1.7 Solids-water partitioning in sewage treatment plant

Table III-186 *Fraction of organic carbon of solids in various STP sludges.*

Parameter	**Symbol**	**Unit**	**Value**
Fraction of organic carbon in solids raw sewage	Foc_{RS}	$[kg_{oc}.kg_{solids}^{-1}]$	0.3
Fraction of organic carbon in solids primary settler	Foc_{PS}	$[kg_{oc}.kg_{solids}^{-1}]$	0.3
Fraction of organic carbon in solids activated sludge	Foc_{A}	$[kg_{oc}.kg_{solids}^{-1}]$	0.37
Fraction of organic carbon in solids in solids-liquid separator	Foc_{SLS}	$[kg_{oc}.kg_{solids}^{-1}]$	0.37

The solids-water partition coefficients for various STP sludges are estimated from *Koc*.

$$Kp_i = Foc_i \cdot Koc \qquad i \in \{RS, PS, A, SLS\} \qquad (632)$$

Input

Koc	organic carbon-water partition coefficient	$[m^3.kg^{-1}]$	O
Foc_{RS}	fraction of organic carbon in raw sewage sludge	$[kg.kg^{-1}]$	D
Foc_{PS}	fraction of organic carbon in settled sewage sludge	$[kg.kg^{-1}]$	D
Foc_{A}	fraction of organic carbon in activated sewage sludge	$[kg.kg^{-1}]$	D
Foc_{SLS}	fraction of organic carbon in effluent sewage sludge	$[kg.kg^{-1}]$	D

Output

Kp_{RS}	solids-water partition coeff. in raw sewage sludge	$[m^3.kg^{-1}]$	O
Kp_{PS}	solids-water partition coeff. in settled sewage sludge	$[m^3.kg^{-1}]$	O
Kp_{A}	solids-water partition coeff. in activated sewage sludge	$[m^3.kg^{-1}]$	O
Kp_{SLS}	solids-water partition coeff. in effluent sewage sludge	$[m^3.kg^{-1}]$	O

In the absence of better adsorption/ desorption data, the results from the Zahn-Wellens elimination level can be used as an estimate of the extent of adsorption to sludge (the 3^h – value is recommended). Especially for water soluble and highly adsorptive substances this is recommended in the TGD (Part II; EC, 2003).

III.4.1.8 Total compartment-water partitioning

Kp describes the partitioning between solids and water in a compartment. The 'dimensionless' form of *Kp*, or the total compartment-water partition coefficient, is derived from the definition of the compartments in three phases.

$$K_{soil-water} = Fair_{soil} \cdot K_{air-water} + Fwater_{soil} + Fsolid_{soil} \cdot Kp_{soil} \cdot RHOsolid \qquad (633)$$

$$K_{susp-water} = Fwater_{susp} + Fsolid_{susp} \cdot Kp_{susp} \cdot RHOsolid \qquad (634)$$

$$K_{sed-water} = Fwater_{sed} + Fsolid_{sed} \cdot Kp_{sed} \cdot RHOsolid \qquad (635)$$

Input			
$Fwater_{soil}$	fraction of water in soil	[$m^3.m^{-3}$]	D
$Fsolid_{soil}$	fraction of solids in soil	[$m^3.m^{-3}$]	D
$Fair_{soil}$	fraction of air in soil	[$m^3.m^{-3}$]	D
$Fwater_{sed}$	fraction of water in sediment	[$m^3.m^{-3}$]	D
$Fsolid_{sed}$	fraction of solids in sediment	[$m^3.m^{-3}$]	D
$Fwater_{susp}$	fraction of water in suspended matter	[$m^3.m^{-3}$]	D
$Fsolid_{susp}$	fraction of solids in suspended matter	[$m^3.m^{-3}$]	D
RHOsolid	density of solid phase	[$kg.m^{-3}$]	D
Kp_{soil}	solids-water partition coefficient in soil	[$m^3.kg^{-1}$]	O
Kp_{sed}	solids-water partition coefficient in sediment	[$m^3.kg^{-1}$]	O
Kp_{susp}	solids-water partition coefficient in suspended matter	[$m^3.kg^{-1}$]	O
$K_{air-water}$	air-water partition coefficient	[$m^3.m^{-3}$]	O^c
Output			
$K_{soil-water}$	total soil-water partition coefficient	[$m^3.m^{-3}$]	O^c
$K_{susp-water}$	total suspended matter-water partition coefficient	[$m^3.m^{-3}$]	O^c
$K_{sed-water}$	total sediment-water partition coefficient	[$m^3.m^{-3}$]	O^c

III.4.2 Degradation and transformation rates

Since measured data on degradation processes for different compartments are not usually available, they must be extrapolated from standardised laboratory tests. In this section, degradation rate constants are derived for abiotic degradation in surface water (hydrolysis and photolysis) and biotic degradation (in soil, sediment, water and sewage treatment). Abiotic degradation in marine environments should be assessed in a similar manner to abiotic degradation in freshwater environments except that the different physico-chemical conditions in marine environments should be taken into account. Abiotic degradation is not estimated for the compartments soil, sediment and STP. If rate constants are known, their default setting of zero (see table below) may be changed.

Input		
	characterisation of biodegradability (ready/inherent/non-biodegradable/specific criteria)	
TEMPtest	temperature of the measured data in standard/simulation test	[K]
$DT50hydr_{water\_temp\ test}$	half-life for hydrolysis in water at the temperature of the data set	[d]
$DT50photo_{water}$	half-life for photolysis in water	[d]
k_{OH}	specific degradation rate constant with OH-radicals	$[m^3.molec^{-1}.d^{-1}]$
$DT50bio_{water\_temp\ test}$	half-life for biodegradation in water at temperature of the data set	[d]
$DT50bio_{soil\_temp\ test}$	half-life for biodegradation in soil at temperature of data set	[d]
$DT50bio\text{-}aer_{sed\_temp\ test}$	half-life for biodeg. in aerobic sediment at temperature of data set	[d]
Intermediate results		
$DT50hydr_{water\_temp\ env}$	half-life for hydrolysis in water at the environmental temperature	[d]
$DT50bio_{stp}$	half-life for biodegradation in STP	[d]
$DT50bio_{water}$	half-life for biodegradation in bulk surface water	[d]
$DT50bio_{water\_temp\ env}$	half-life for biodegradation in water at the environmental temp.	[d]
$DT50bio_{soil}$	half-life for biodegradation in bulk soil	[d]
$DT50bio_{soil\_temp\ env}$	half-life for biodegradation in soil at the environmental temp.	[d]
$DT50bio\text{-}aer_{sed}$	half-life for biodegradation in aerobic sediment	[d]
$DT50bio\text{-}aer_{sed\_temp\ env}$	half-life for biodeg. in aerobic sediment at environmental temp.	[d]
Output		
$kdeg_{air}$	total rate constant for degradation in air	$[d^{-1}]$
$kdeg_{stp}$	total rate constant for degradation in STP	$[d^{-1}]$
$kdeg_{water}$	total rate constant for degradation in bulk surface water	$[d^{-1}]$
$kdeg_{soil}$	total rate constant for biodegradation in bulk soil	$[d^{-1}]$
$kdeg_{sed}$	total rate constant for biodegradation in bulk sediment	$[d^{-1}]$

Table III-187 *Defaults for calculating degradation rates.*

Parameter	Symbol	Unit	Value
Concentration of OH-radicals in atmosphere	$OHCONC_{air}$	$[molecules.m^{-3}]$	5.10^{11}
Fraction of sediment compartment that is aerated	$Faer_{sed}$	$[m^3.m^{-3}]$	0.10
Rate constant for abiotic degradation in STP	$kabio_{stp}$	$[d^{-1}]$	0
Rate constant for abiotic degradation in soil	$kabio_{soil}$	$[d^{-1}]$	0
Rate constant for abiotic degradation in sediment	$kabio_{sed}$	$[d^{-1}]$	0
Rate constant for anaerobic biodegr. in sediment	$kbio\text{-}anaer_{sed}$	$[d^{-1}]$	0
Environmental temperature	TEMP	[K]	
Freshwater environment (12 °C)			285
Marine environment (12 °C)			285 [a]

[a] Although the TGD (2003) proposed a temperature of 9 °C, due to the small differences it was decided to keep the temperature the same for all compartments on the moderate global scale the same.

III.4.2.1 Hydrolysis in water

Rates of hydrolysis increases with increasing temperature. When hydrolysis half-lives have been determined in standard tests, they should be recalculated to reflect an average EU outdoor temperature by the equation:

$$DT50hydr_{water\_temp\,env} = DT50hydr_{water\_temp\,test} \cdot e^{(0.08 \cdot (TEMPtest - TEMPenv))}$$

Input

$DT50hydr_{water\_temp\ test}$	half-life for hydrolysis in water at the temperature of the data set	[d]	S
TEMPtest	temperature of the measured data in standard test	[K]	S
TEMP	environmental temperature	[K]	D
Output			
$DT50hydr_{water\_temp\ env}$	half-life for hydrolysis in water at the environmental temperature	[d]	O

Values for the half-life (DT50) of a hydrolysable substance (if known) can be converted to degradation rate constants, which are used in the distribution models.

$$khydr_{water} = \frac{\ln 2}{DT50\,hydr_{water\_temp\,env}} \qquad (636)$$

Input

$DT50hydr_{water\_temp\ env}$	half-life for hydrolysis in water at the environmental temperature	[d]	O
Output			
$khydr_{water}$	rate constant for hydrolysis in water	[d^{-1}]	O

III.4.2.2 Photolysis in surface water

A value for the half-life for photolysis in water (if known) can be converted to a first-order rate constant.

$$kphoto_{water} = \frac{\ln 2}{DT\,50\,photo_{water}} \qquad (637)$$

Input

$DT50photo_{water}$	half-life for photolysis in water	[d]	S
Output			
$kphoto_{water}$	rate constant for photolysis in water	[d^{-1}]	O

III.4.2.3 Photochemical reactions in the atmosphere

Although for some chemicals direct photolysis may be an important breakdown process, for most substances, the most effective elimination process in the troposphere is reaction with photochemically generated species like OH-radicals, ozone and nitrate radicals. The specific degradation rate constant of a substance with OH-radicals can either be determined experimentally (OECD, 1992c) or estimated by (Q)SAR-methods (see Chapter 4 of the TGD). By relating k_{OH} to the OH-radical concentration in the atmosphere, the pseudo-first-order rate constant in air is determined:

$$k\deg_{air} = k_{OH} \cdot OHCONC_{air} \tag{638}$$

Input

k_{OH}	specific degradation rate constant with OH-radicals	[$m^3.molec^{-1}.d^{-1}$]	S
$OHCONC_{air}$	concentration of OH-radicals in atmosphere	[$molecules.m^{-3}$]	D

Output

$kdeg_{air}$	rate constant for degradation in air	[d^{-1}]	O

III.4.2.4 Biodegradation in the sewage treatment plant

For the purpose of modelling a sewage treatment plant (STP), the rate constants of Table III-188 have been derived to extrapolate from the biodegradation screening tests.

Table III-188 *Elimination in sewage treatment plants: extrapolation from test results to rate constants in the STP model (SimpleTreat).*

Test result	**Rate constant (hr^{-1})**	**Rate constant (d^{-1})**	**Half-life (d)**
		$kbio_{stp}$	$DT50bio_{stp}$
Readily biodegradable	1	24	0.029
Readily biodegradable, but failing 10-d window	0.3	7.2	0.096
Inherently biodegradable, fulfilling specific criteria	0.1	2.4	0.29
Inherently biodegradable, not fulfilling specific criteria	0	0	∞
Not biodegradable	0	0	∞

Specific criteria that the various inherent biodegradation tests must fulfil:

Zahn-Wellens test:	Pass level must be reached within 7 days, log-phase (time window) should be no longer than 3 days, percentage removal in the test before biodegradation occurs should be below 15 %.
MITI-II test:	Pass level must be reached within 14 days, log-phase (time window) should be no longer than 3 days.

No specific criteria have been developed for positive results in a SCAS test. A rate constant of 0 d^{-1} is assigned to a substance, irrespective of whether it passes this test or not.

Table III-188 gives the following input-output:

Input

	results of screening test on biodegradability		P
Output			
$kbio_{stp}$	rate constant for biodegradation in STP	$[d^{-1}]$	O
$DT50bio_{stp}$	half-life for biodegradation in STP	[d]	O

The overall degradation-rate constant is given by:

$$k\deg_{stp} = kbio_{stp} + kabio_{stp} \tag{639}$$

Input

$kbio_{stp}$	rate constant for biodegradation in STP	$[d^{-1}]$	O
$kabio_{stp}$	rate constant for abiotic degradation in STP	$[d^{-1}]$	D
Output			
$kdeg_{stp}$	rate constant for degradation in STP	$[d^{-1}]$	O

III.4.2.5 Biodegradation in surface water

The table below gives half-lives for biodegradation in bulk surface water (freshwater and marine), based on the results of screening tests for biodegradability.

Table III-189 *Half-lives for biodegradation in bulk surface water (freshwater and marine) at the environmental temperature, based on results of screening tests on biodegradability.*

Test result	**Half-life for biodegradation in bulk surface water (d)** $DT50bio_{water}$		
	Freshwater	**Estuaries**[a]	**Other marine environments**[b]
Degradable in marine screening test	n.a.	15	50
Readily biodegradable	15	15	50
Readily biodegradable, but failing 10-d window	50	50	150
Inherently biodegradable	150	150	∞
Persistent	∞	∞	∞

n.a. Not applicable

[a] Also including shallow marine water closest to the coastline

[b] The half lives mentioned under this heading are normally to be used in the regional assessement (coastal model)

Input

	results of screening test on biodegradability		P
Output			
$DT50bio_{water}$	half-life for biodegradation in bulk surface water	[d]	O

Temperature influences the activity of micro-organisms and thus the biodegradation rate in the environment. When biodegradation rates or half-lives have been determined in simulation tests, it should be considered to recalculate the degradation rates obtained to reflect an average EU outdoor temperature by the following equation:

$$DT50bio_{water\_temp\,env} = DT50bio_{water\_temp\,test} \cdot e^{(0.08 \cdot (TEMPtest - TEMPenv))} \qquad \mathbf{(640)}$$

Input			
$DT50bio_{water\_temp\,test}$	half-life for biodegradation in water at temperature of the data set	[d]	S
TEMPtest	temperature of the measured data in simulation test	[K]	S
TEMP	environmental temperature	[K]	D
Output			
$DT50bio_{water\_temp\,env}$	half-life for biodegradation in water at the environmental temp.	[d]	O

Values for the half-life (DT50) for biodegradation can be converted to first order rate constants for biodegradation.

$$kbio_{water} = \frac{\ln 2}{DT50\,bio_{water}} \quad or \quad kbio_{water} = \frac{\ln 2}{DT50\,bio_{water\_temp\,env}} \qquad \mathbf{(641)}$$

Input			
$DT50bio_{water}$	half-life for biodegradation in bulk surface water	[d]	O
$DT50bio_{water\_temp\,env}$	half-life for biodegradation in water at the environmental temp.	[d]	O
Output			
$kbio_{water}$	rate constant for biodegradation in bulk surface water	[d^{-1}]	O

III.4.2.6 Overall rate constant for degradation in bulk surface water

The rate constants for the various different transformation processes can be summed into one overall degradation rate constant (used for regional and continental calculations only). It should be noted that different types of degradation (primary and ultimate) are added, which is done for modelling purposes only.

$$k\deg_{water} = khydr_{water} + kphoto_{water} + kbio_{water} \qquad \mathbf{(642)}$$

Input			
$khydr_{water}$	rate constant for hydrolysis in surface water	[d^{-1}]	O
$kphoto_{water}$	rate constant for photolysis in surface water	[d^{-1}]	O
$kbio_{water}$	rate constant for biodegradation in bulk surface water	[d^{-1}]	O
Output			
$kdeg_{water}$	total rate constant for degradation in bulk surface water	[d^{-1}]	O

III.4.2.7 Biodegradation in soil and sediment

In Table III-190 rate constants are given for degradation in bulk soil. Since it is assumed that no degradation takes place in the bound phase, the rate constant in principle depends on the partition coefficient of the chemical.

Table III-190 *Half-lives for (bulk) soil and aerobic sediment, based on results from standardised biodegradation tests.*

	Half-life for soil and aerobic sediment (d) [a] $DT50bio_{soil}$ / $DT50bio\text{-}aer_{sed}$ [b]		
Kp_{soil} / Kp_{sed} [b] $[m^3.kg^{-1}]$	Readily biodegradable	Readily biodegradable, failing 10-d window	Inherently biodegradable
≤ 0.1	30	90	300
>0.1, ≤ 1.0	300	900	3000
>1.0, ≤ 10	3000	9000	30000
etc.	etc.	etc.	etc.

a In the case of non-biodegradable substances an infinite half-life is assumed.

b For deriving the degradation rate in aerobic sediment, the same half-life as for soil is used, but using the *Kp* for sediment.

Input

	results of screening test on biodegradability		P
Kp_{soil}	solids-water partition coefficient in soil	$[m^3.kg^{-1}]$	O
Output			
$DT50bio_{soil}$	half-life for biodegradation in bulk soil	[d]	O
$DT50bio\text{-}aer_{sed}$	half-life for biodegradation in aerobic sediment	[d]	O

Temperature influences the activity of micro-organisms and thus the biodegradation rate in the environment. When biodegradation rates or half-lives have been determined in simulation tests, it should be considered to recalculate the degradation rates obtained to reflect an average EU outdoor temperature by the following equations:

$$DT50bio_{soil\_temp\,env} = DT50bio_{soil\_temp\,test} \cdot e^{(0.08 \cdot (TEMPtest - TEMPenv))} \qquad \textbf{(643)}$$

$$DT50bio - aer_{sed\_temp\,env} = DT50bio - aer_{sed\_temp\,test} \cdot e^{(0.08 \cdot (TEMPtest - TEMPenv))} \qquad \textbf{(644)}$$

Input			
$DT50bio_{soil\_temp\ test}$	half-life for biodegradation in soil at temperature of data set	[d]	S
$DT50bio\text{-}aer_{sed\_temp\ test}$	half-life for biodeg. in aerobic sediment at temperature of data set	[d]	O
TEMPtest	temperature of the measured data in simulation test	[K]	S
TEMP	environmental temperature	[K]	D
Output			
$DT50bio_{soil\_temp\ env}$	half-life for biodegradation in soil at the environmental temp.	[d]	O
$DT50bio\text{-}aer_{sed\_temp\ env}$	half-life for biodeg. in aerobic sediment at environmental temp.	[d]	O

The following equation converts the DT50 to a rate constant for biodegradation in bulk soil. A rate constant for abiotic degradation (if known) is added.

$$kbio_{soil} = \frac{\ln 2}{DT50bio_{soil}} \quad or \quad kbio_{soil} = \frac{\ln 2}{DT50bio_{soil\_temp\ env}} \tag{645}$$

$$k\deg_{soil} = kbio_{soil} + kabio_{soil} \tag{646}$$

Input			
$DT50bio_{soil}$	half-life for biodegradation in bulk soil	[d]	O
$DT50bio_{soil\_temp\ env}$	half-life for biodegradation in soil at the environmental temp.	[d]	O
$kabio_{soil}$	rate constant for abiotic degradation in bulk soil	[d^{-1}]	D
$kbio_{soil}$	rate constant for biodegradation in bulk soil	[d^{-1}]	O
Output			
$kdeg_{soil}$	total rate constant for degradation in bulk soil	[d^{-1}]	O

The extrapolation of test results to rate constants for sediment is problematic, given the fact that sediment generally consists of a relatively thin oxic top layer and anoxic deeper layers. For the degradation in the anoxic layers, a rate constant of zero (infinite half-life) is assumed unless specific information on degradation under anaerobic conditions is available. For the oxic zone, the same rate constant and temperature correction as that for soil is assumed (see Table III-190).

$$kbio_{aer-sed} = \frac{\ln 2}{DT50bio - aer_{sed}} \quad or \quad kbio_{aer-sed} = \frac{\ln 2}{DT50bio - aer_{sed\_temp\ env}} \tag{647}$$

$$k\,deg_{sed} = Faer_{sed} \cdot kbio - aer_{sed} + (1 - Faer_{sed}) \cdot kbio - anaer_{sed} + kabio_{sed} \tag{648}$$

Input			
$DT50bio\text{-}aer_{sed}$	half-life for biodegradation in aerobic sediment	[d]	O
$DT50bio\text{-}aer_{sed\_temp\ env}$	half-life for biodeg. in aerobic sediment at environmental temp.	[d]	O
$Faer_{sed}$	fraction of sediment compartment that is aerated	[$m^3.m^{-3}$]	D
$kabio_{sed}$	rate constant for abiotic degradation in bulk sediment	[d^{-1}]	D
$kbio\text{-}anaer_{sed}$	rate constant for anaerobic biodegradation in sediment	[d^{-1}]	D
Output			
$kbio\text{-}aer_{sed}$	rate constant for biodegradation in aerobic sediment	[d^{-1}]	O
$kdeg_{sed}$	total rate constant for degradation in bulk sediment	[d^{-1}]	O

III.4.3 Sewage treatment

Emissions to wastewater are treated in a sewage treatment plant (STP). For estimation of fate in an STP, the model SimpleTreat 3.1is used, which differs from version 3.0 only with respect to the default calculation of the solids-water partitioning coefficient Kp. This model is not described in detail in this section. For details and the mathematical process descriptions, the reader is referred to the SimpleTreat reference manual (Struijs, 1996). Sewage treatment takes place at the local, regional and continental scale. The definition of STP characteristics is the same at each of these spatial scales. The number of inhabitants is used to scale the size of the STP.

The following options are included in the STP module:

- temperature dependence of biodegradation,
- Monod degradation kinetics,
- not considering a primary settler (this 'six-box option' can only be specified at the local spatial scale).

Input: chemical properties			
HENRY	Henry's law constant	$[Pa.m^3.mol^{-1}]$	
$kdeg_{stp}$	total rate constant for degradation in STP	$[d^{-1}]$	
Kp_{RS}	solids-water partition coeff. in raw sewage sludge	$[m^3.kg^{-1}]$	
Kp_{PS}	solids-water partition coeff. in settled sewage sludge	$[m^3.kg^{-1}]$	
Kp_A	solids-water partition coeff. in activated sewage sludge	$[m^3.kg^{-1}]$	
Kp_{SLS}	solids-water partition coeff. in effluent sewage sludge	$[m^3.kg^{-1}]$	
Input: emissions			
$Elocal_{water}$	local emission rate to wastewater during episode	$[kg_c.d^{-1}]$	
$Ereg_{water}$	regional emission rate to wastewater (annual average)	$[kg_c.d^{-1}]$	
$Econt_{water}$	continental emission rate to wastewater (annual average)	$[kg_c.d^{-1}]$	
Intermediate results			
$EFFLUENTlocal_{stp}$	effluent discharge rate of local STP	$[m^3.d^{-1}]$	c
$Fstp_i$	fraction directed to compartment *i* by local STP	[-]	
$Fstp\text{-}reg_i$	fraction directed to compartment *i* by regional STP	[-]	
$Fstp\text{-}cont_i$	fraction directed to compartment *i* by continental STP	[-]	
	$i \in$ {air,water,sludge,degr}		
Output: local			
$Estp_{air}$	local indirect emission to air from STP during episode	$[kg_c.d^{-1}]$	
$Clocal_{eff}$	concentration of chemical (total) in the STP effluent	$[kg_c.m^{-3}]$	
C_{sludge}	concentration in dry sewage sludge	$[kg_c.kg^{-1}]$	
PEC_{stp}	PEC for micro-organisms in STP	$[kg_c.m^{-3}]$	
Output: regional			
$Estp\text{-}reg_{air}$	regional indirect emission to air from STP	$[kg_c.d^{-1}]$	
$Estp\text{-}reg_{water}$	regional indirect emission to surface water from STP	$[kg_c.d^{-1}]$	
$Estp\text{-}reg_{agric}$	regional indirect emission to agricultural soil via sludge	$[kg_c.d^{-1}]$	
Output: continental			
$Estp\text{-}cont_{air}$	continental indirect emission to air from STP	$[kg_c.d^{-1}]$	
$Estp\text{-}cont_{water}$	continental indirect emission to surface water from STP	$[kg_c.d^{-1}]$	
$Estp\text{-}cont_{agric}$	continental indirect emission to agricultural soil via sludge	$[kg_c.d^{-1}]$	

Table III-191 lists the fixed parameters, subdivided into the categories raw sewage, primary sedimentation (9-box only), aerator and solids-liquid separation.

Table III-191 *Fixed parameters for raw sewage and the operation of domestic wastewater treatment.*

Parameter	**Symbol**	**Unit**	**Value**
raw sewage			
Mass of O_2-binding material per person per day	BOD	$[kg_{O2}.eq^{-1}.d^{-1}]$	0.054
Dry weight of solids produced per person per day	SOLIDS	$[kg_{dwt}.eq.^{-1}\ d^{-1}]$	0.09
Density of solids	RHO_{RS}	$[kg_{dwt}.m^{-3}]$	1500
primary settler (9-box only)			
Depth	$DEPTH_{PS}$	[m]	4
Hydraulic retention time (2 hours)	HRT_{PS}	[d]	0.083
Density of suspended and settled solids	RHO_{PS}	$[kg_{dwt}.m^{-3}]$	1500
activated sludge tank			
Depth	$DEPTH_A$	[m]	3
Density solids of activated sludge	RHO_A	$[kg_{dwt}.m^{-3}]$	1300
Concentration solids of activated sludge	CAS	$[kg_{dwt}.m^{-3}]$	4
Steady-state O_2 concentration in activated sludge	COX	$[kg.m^{-3}]$	0.002
Aeration rate of bubble aeration	G	$[m^3.d^{-1}.eq^{-1}]$	1.13
solids-liquid separator			
Depth	$DEPTH_{SLS}$	[m]	3
Density of suspended and settled solids	RHO_{SLS}	$[kg_{dwt}.m^{-3}]$	1300
Concentration of solids in effluent	$SUSP_{eff}$	$[kg_{dwt}.m^{-3}]$	0.03
Hydraulic retention time (6 hours)	HRT_{SLS}	[d]	0.25

Only four parameters may be specified if the user does not accept the default values (see Table III-192). The sludge loading-rate parameter, k_{SLR} (kg BOD kg_{dwt}^{-1} d^{-1}), is chosen instead of the sludge retention time, SRT (d), to quantify the BOD loading of the installation. In principle, the hydraulic retention time, HRT (hr), could also have been chosen for this purpose. For the operation range relevant for wastewater treatment technology, these three parameters are interdependent according to certain relationships, which in some cases are empirical.

Table III-192 *Input parameters characterising size and mode of operation of sewage treatment plant.*

Parameter	**Symbol**	**Units**	**Value**
Sewage flow	Q_{stp}	$[m^3.eq^{-1}.d^{-1}]$	0.2
Number of inhabitants feeding system at scale local region EU	Nlocal N *	[eq]	10000 20.10^6 370.10^6
Sludge-loading rate	k_{SLR}	$[kg_{BOD}.kg_{dwt}^{-1}.d^{-1}]$	0.15
Temperature of air above aeration tank (15 °C)	$TEMPstp_{air}$	[K]	288
Temperature of water in aeration tank (15 °C)	$TEMPstp_{water}$	[K]	288
Wind speed (3 m/s)	WINDSPEED	$[m.d^{-1}]$	$2.59.10^5$
Mode of aeration: surface (s) or bubble aeration (b)	M	[-]	s

* Different parameter value possible on regional and continental scale.

III.4.3.1 STP calculations

The SimpleTreat calculations yield the following input-output:

Input			
HENRY	Henry's law constant	$[Pa.m^3.mol^{-1}]$	O
$kdeg_{stp}$	rate constant for biodegradation in STP	$[d^{-1}]$	O
$Elocal_{water}$	local emission rate to wastewater during episode	$[kg_c.d^{-1}]$	O
$Ereg_{water}$	regional emission rate to wastewater (annual average)	$[kg_c.d^{-1}]$	O
$Econt_{water}$	continental emission rate to wastewater (annual average)	$[kg_c.d^{-1}]$	O
Kp_{RS}	solids-water partition coeff. in raw sewage sludge	$[m^3.kg^{-1}]$	O
Kp_{PS}	solids-water partition coeff. in settled sewage sludge	$[m^3.kg^{-1}]$	O
Kp_A	solids-water partition coeff. in activated sewage sludge	$[m^3.kg^{-1}]$	O
Kp_{SLS}	solids-water partition coeff. in effluent sewage sludge	$[m^3.kg^{-1}]$	O
Output			
$Clocal_{eff}$	concentration of chemical (total) in STP effluent	$[kg_c.m^{-3}]$	O
C_{sludge}	concentration in dry sewage sludge	$[kg_c.kg_{dwt}^{-1}]$	O
$Fstp_i$	fraction of emission directed to compartment *i* by STP	[-]	O
$Fstp\text{-}reg_i$	fraction directed to compartment *i* by regional STP	[-]	O
$Fstp\text{-}cont_i$	fraction directed to compartment *i* by continental STP	[-]	O
	$i \in \{air,water,sludge,degr\}$		

EUSES will perform a check whether the effluent concentration ($Clocal_{eff}$) exceeds the water solubility. If this is the case, the results of this module should be studied in more detail on a case-by-case basis.

III.4.3.2 Calculation of influent concentration

The influent concentration is used for exposure of micro-organisms in the case of intermittent release. For local-scale assessments, it is assumed that one point source is releasing its wastewater to one STP. The concentration in the influent of the STP, i.e. the untreated wastewater, can be calculated from the local emission to wastewater and the influent discharge of the STP. The influent discharge equals the effluent discharge.

$$Clocal_{inf} = \frac{Elocal_{water}}{EFFLUENTlocal_{stp}} \qquad (649)$$

$$Clocal_{eff} = Clocal_{\text{inf}} \cdot Fstp_{water} \qquad (650)$$

Input			
$Elocal_{water}$	local emission rate to wastewater during episode	[$kg_c.d^{-1}$]	O
$EFFLUENTlocal_{stp}$	effluent discharge rate of local STP	[$m^3.d^{-1}$]	O^c
$Fstp_{water}$	fraction of the emission to wastewater directed to effluent	[-]	O
Output			
$Clocal_{inf}$	concentration in untreated wastewater	[$kg_c.m^{-3}$]	O
$Clocal_{eff}$	concentration of chemical in the STP effluent	[$kg_c.m^{-3}$]	O

For calculating the PEC in surface water (fresh water or marine water) without sewage treatment, the fraction of the emission to wastewater directed to effluent ($Fstp_{water}$) should be set to 1. The fractions to air and sludge ($Fstp_{air}$ and $Fstp_{sludge}$, respectively) should be set to zero. This ($Fstp_{water}$=1) is the default for local emissions to the marine environment.

The effluent discharge of the local STP is given by the following equation. The effluent discharges of the regional and continental STPs are given in Section III.4.4.5 (Equation 127 and 119 MOET DIT NIET ZIJN 655 and 656????). It should be noted that measured effluent-discharge rates cannot be entered directly by the user, but have to be derived by adjusting the number of inhabitants and the sewage flow per inhabitant.

$$EFFLUENTlocal_{stp} = Nlocal \cdot Q_{stp} \qquad (651)$$

Input			
Nlocal	capacity of the local STP, number of inhabitants	[eq]	D
Q_{stp}	sewage flow per inhabitant	[$m^3.d^{-1}.eq^{-1}$]	D
Output			
$EFFLUENTlocal_{stp}$	effluent discharge rate of local STP	[$m^3.d^{-1}$]	O^c

III.4.3.3 PEC for micro-organisms in STP

For the risk characterisation of a chemical for micro-organisms in the STP, ideally the concentration in the aeration tank should be used. Assuming homogeneous mixing in the aeration tank, the dissolved concentration of a substance there is equal to the effluent concentration:

$$PEC_{stp} = Clocal_{eff} \qquad (652)$$

Input			
$Clocal_{eff}$	total concentration of chemical in STP effluent	$[kg_c.m^{-3}]$	O
Output			
PEC_{stp}	PEC for micro-organisms in STP	$[kg_c.m^{-3}]$	O

However, in the case of intermittent release, the concentration in of STP influent is more representative because the highest concentration as a result of shock load is accounted for.

$$PEC_{stp} = Clocal_{inf} \qquad (653)$$

Input			
$Clocal_{inf}$	total concentration of chemical in STP influent	$[kg_c.m^{-3}]$	O
Output			
PEC_{stp}	PEC for micro-organisms in STP	$[kg_c.m^{-3}]$	O

III.4.3.4 Calculation of the emission to air from the STP

The (indirect) emission from the STP to air is given by the fraction of the emission to wastewater, directed to air.

$$Estp_{air} = Fstp_{air} \cdot Elocal_{water} \qquad (654)$$

Input			
$Fstp_{air}$	fraction of emission to air from STP	[-]	O
$Elocal_{water}$	local emission rate to wastewater during emission episode	$[kg_c.d^{-1}]$	O
Output			
$Estp_{air}$	local emission to air from STP during emission episode	$[kg_c.d^{-1}]$	O

III.4.3.5 Emissions from STP at the regional and continental scale

The indirect emissions via the STP at the regional and continental scale are calculated from the emissions to wastewater and the fate in the STP. The relative fate (expressed as fractions redirected to air, water and sludge) will usually be identical at all three spatial scales. However, when the degradation in the STP is modelled by Monod kinetics, differences in fate are possible.

$$Estp\text{-}reg_i = Fstp\text{-}reg_i \cdot Ereg_{water} \qquad (655)$$

$$Estp\text{-}cont_i = Fstp\text{-}cont_i \cdot Econt_{water} \qquad (656)$$

$$i \in \{air, water, sludge/agric\}$$

Input

Fstp-reg$_i$	fraction directed to compartment *i* by regional STP	[-]	O
Fstp-cont$_i$	fraction directed to compartment *i* by continental STP	[-]	O
Ereg$_{water}$	regional emission rate to wastewater	[kg$_c$.d^{-1}]	O
Econt$_{water}$	continental emission rate to wastewater	[kg$_c$.d^{-1}]	O

Output

Estp-reg$_{air}$	regional emission to air from STP	[kg$_c$.d^{-1}]	O
Estp-reg$_{water}$	regional emission to water from STP	[kg$_c$.d^{-1}]	O
Estp-reg$_{agric}$	regional emission to agricultural soil via sludge	[kg$_c$.d^{-1}]	O
Estp-cont$_{air}$	continental emission to air from STP	[kg$_c$.d^{-1}]	O
Estp-cont$_{water}$	continental emission to water from STP	[kg$_c$.d^{-1}]	O
Estp-cont$_{agric}$	continental emission to agricultural soil via sludge	[kg$_c$.d^{-1}]	O

III.4.4 Regional environmental distribution

Steady-state exposure concentrations at the regional and continental scales are calculated for all environmental compartments using a nested version of the multi-media fate model SimpleBox (Van de Meent, 1993; Brandes *et al.*, 1996; see also Section 2.4.4). The version of SimpleBox implemented in EUSES is described in technical detail by den Hollander, van de Meent and van Eijkeren (2003, in prep.) In this section, the regional model is described by its inputs, outputs and default values. Furthermore, the calculations for the net sedimentation rate and the residence time in air and water are given (these are shown as closed outputs in the defaults section of the EUSES programme).

Input: regional emissions

$Ereg_{j}$	direct emission to compartment *j* (annual average flux) $j \in$ {direct-water,ind,agric,air}	$[kg_{c}.d^{-1}]$	
$Estp\text{-}reg_{j}$	regional indirect emission to compartment *j* from STP $j \in$ {water,agric,air}	$[kg_{c}.d^{-1}]$	

Input: continental emissions

$Econt_{j}$	direct emission to compartment *j* (annual average flux) $j \in$ {direct-water,ind,agric,air}	$[kg_{c}.d^{-1}]$	
$Estp\text{-}cont_{j}$	continental indirect emission to compartment *j* from STP $j \in$ {water,agric,air}	$[kg_{c}.d^{-1}]$	

Input: chemical properties

Kow	octanol-water partition coefficient (only for estimation of BCF for aquatic biota)	[S]	
$Fass_{aer}$	fraction of chemical associated with aerosol particles	[-]	
$K_{air-water}$	air-water partition coefficient	$[m^{3}.m^{-3}]$	c
$K_{soil-water}$	soil-water partition coefficient	$[m^{3}.m^{-3}]$	c
$K_{sed-water}$	sediment-water partition coefficient	$[m^{3}.m^{-3}]$	c
Kp_{susp}	solids-water partition coefficient in suspended matter	$[m^{3}.kg_{solids}^{-1}]$	
RHO_{soil}	wet bulk density of soil	$[kg_{wwt}.m^{-3}]$	c
$kdeg_{air}$	rate constant for degradation in air	$[d^{-1}]$	
$kdeg_{water}$	rate constant for degradation in bulk water	$[d^{-1}]$	
$kdeg_{soil}$	rate constant for degradation in bulk soil	$[d^{-1}]$	
$kdeg_{sed}$	rate constant for degradation in bulk sediment	$[d^{-1}]$	

Output: continental concentrations

$PECcont_{water,tot}$	continental PEC in surface water (total)	$[kg_{c}.m^{-3}]$	c
$PECcont_{water}$	continental PEC in surface water (dissolved)	$[kg_{c}.m^{-3}]$	c
$PECcont_{air}$	continental PEC in air (total)	$[kg_{c}.m^{-3}]$	c
$PECcont_{agric}$	continental PEC in agricultural soil (total)	$[kg_{c}.kg_{wwt}^{-1}]$	c
$PECcont_{agric,porew}$	continental PEC in pore water of agricultural soils	$[kg_{c}.m^{-3}]$	c
$PECcont_{natural}$	continental PEC in natural soil (total)	$[kg_{c}.kg_{wwt}^{-1}]$	c
$PECcont_{ind}$	continental PEC in industrial soil (total)	$[kg_{c}.kg_{wwt}^{-1}]$	c
$PECcont_{sed}$	continental PEC in sediment (total)	$[kg_{c}.kg_{wwt}^{-1}]$	c

Output: regional concentrations

$PECreg_{water,tot}$	regional PEC in surface water (total)	$[kg_{c}.m^{-3}]$	
$PECreg_{water}$	regional PEC in surface water (dissolved)	$[kg_{c}.m^{-3}]$	
$PECreg_{air}$	regional PEC in air (total)	$[kg_{c}.m^{-3}]$	
$PECreg_{agric}$	regional PEC in agricultural soil (total)	$[kg_{c}.kg_{wwt}^{-1}]$	
$PECreg_{agric,porew}$	regional PEC in pore water of agricultural soil	$[kg_{c}.m^{-3}]$	
$PECreg_{natural}$	regional PEC in natural soil (total)	$[kg_{c}.kg_{wwt}^{-1}]$	
$PECreg_{ind}$	regional PEC in industrial soil (total)	$[kg_{c}.kg_{wwt}^{-1}]$	
$PECreg_{sed}$	regional PEC in sediment (total)	$[kg_{c}.kg_{wwt}^{-1}]$	

The following tables give the default settings for the regional and continental systems. Most parameter values are taken from the TGD. It should be noted that several characteristic parameters are given in the tables and the TGD which are actually outputs and not defaults: residence time in air and water, and the net sedimentation rate. Therefore, these parameters may change when default values are changed. To comply with the residence times and sedimentation rate of the TGD, several parameters were set to 'not unreasonable values': the fraction of the continental scale water flow that flows into the regional system and the rate of soil erosion.

Table III-193 *General parameter settings for the regional and continental scales.*

Parameter	**Symbol**	**Unit**	**Value**
Area of system (land and sea) region EU	AREA(reg) AREA(EU)	[m^2]	$4.04.10^{10}$ $7.04.10^{12}$
Number of inhabitants region EU	N(reg) N(EU)	[eq]	20.10^{6} [a] 370.10^{6} [a]
Fraction connected to sewer systems	$Fconnect_{stp}$	[-]	0.80 [b]
Per-capita water use	Q_{stp}	[$m^3.d^{-1}$]	0.20 [a]

[a] Already defined in STP sub-module.
[b] Already defined in emission module.

Table III-194 *Default environmental characteristics for local, regional and continental scales*

Parameter	**Symbol**	**Unit**	**Value**
Density of solid phase	RHOsolid	[$kg_{solid}.m_{solid}^{-3}$]	2500 [a]
Volume fraction of solids in sediment (marine and fresh water)	$Fsolid_{sed}$	[$m_{solid}^{3}.m_{sed}^{-3}$]	0.2 [a]
Volume fraction of water in sediment (marine and fresh water)	$Fwater_{sed}$	[$m_{water}^{3}.m_{sed}^{-3}$]	0.8 [a]
Volume fraction of solids in soil	$Fsolid_{soil}$	[$m_{solid}^{3}.m_{soil}^{-3}$]	0.6 [a]
Volume fraction of water in soil	$Fwater_{soil}$	[$m_{water}^{3}.m_{soil}^{-3}$]	0.2 [a]
Volume fraction of air in soil	$Fair_{soil}$	[$m_{air}^{3}.m_{soil}^{-3}$]	0.2 [a]

[a] Already defined in partition coefficients sub-module.

Table III-195 *Parameter settings for regional and continental air.*

Parameter	**Symbol**	**Unit**	**Value**
Atmospheric mixing height	$HEIGHT_{air}$	[m]	1000
Wind speed of system	WINDSPEED	$[m.d^{-1}]$	$2.59.10^{5}$ [a]
Residence time of air region continent	TAU_{air} *	[d]	0.687 O[c] 9.05 O[c]
Aerosol-deposition velocity	$DEPRATE_{aer}$	$[m.d^{-1}]$	86.4
Aerosol-collection efficiency	$COLLEFF_{aer}$	[-]	2.10^{5}
Average daily precipitation	RAINRATE	$[m.d^{-1}]$	$1.92.10^{-3}$

[a] Already defined in STP sub-module.
* Different parameter value possible on regional and continental scale.

Table III-196 *Parameter settings for regional and continental marine and fresh waters.*

Parameter	**Symbol**	**Unit**	**Value**
Area fraction of fresh water region (both 3% of land area) continent	F_{water} *	[-]	0.0297 0.015
Area fraction of marine water region continent	$F_{water,marine}$ *	[-]	0.0099 0.5
Water depth fresh water region+cont.	$DEPTH_{water}$ *	[m]	3
Water depth marine region continent	$DEPTH_{water, marine}$ *	[m]	10 200
Fraction of flow from region larger scale continent	$Fflow_{out}$ *	[-]	0.034 0
Residence time of fresh water region continent	TAU_{water} *	[d]	43.3 O[c] 1721 O[c]
Residence time of marine water region continent	$TAU_{water, marine}$ *	[d]	4.04 O[c] 365 O[c]
Suspended-solids conc. region+cont.	$SUSP_{water}$ *	$[kg_{dwt}.m^{-3}]$	0.015 .
Suspended-solids conc. region+cont.	$SUSP_{water, marine}$ *	$[kg_{dwt}.m^{-3}]$	0.005
Concentration of biota (marine and fresh water)	$BIOTA_{water}$	$[kg_{wwt}.m^{-3}]$	0.001
Fraction of rainwater infiltrating in soil	$Finf_{soil}$	[-]	0.25 [a]
Rate of wet precipitation (700 mm/year)	RAINRATE	$[m.d^{-1}]$	$1.92.10^{-3}$ [a]

* Different parameter value possible on regional and continental scale.

Table III-197 *Parameter settings for regional and continental marine and fresh water sediments.*

Parameter	**Symbol**	**Unit**	**Value**
Sediment mixing depth	$DEPTH_{sed}$	[m]	0.03
Settling velocity of suspended solids	$SETTLRATE_{susp}$	$[m.d^{-1}]$	2.5
(Biogenic) production of suspended solids in fresh water region: $10g.m^{-2}.a^{-1}$ continent: $10g.m^{-2}.a^{-1}$	$SUSPPROD_{water}$ *	$[kg.d^{-1}]$	$3.3.10^{4}$ Oc $2.9.10^{6}$ Oc
(Biogenic) production of suspended solids in marine water region: $10g.m^{-2}.a^{-1}$ continent: $5g.m^{-2}.a^{-1}$	$SUSPPROD_{water, marine}$ *	$[kg.d^{-1}]$	$1.1.10^{4}$ Oc $4.8.10^{7}$ Oc
Suspended solids in STP effluent	$SUSP_{eff}$	$[kg_{dwt}.m^{-3}]$	0.030 [a]
Net sedimentation rate fresh water region continent	NETsedrate *	$[m_{sed}.d^{-1}]$	 $7.5.10^{-6}$ O^{c} $7.5.10^{-6}$ O^{c}
Net sedimentation rate marine water region continent	$NETsedrate_{marine}$ *	$[m_{sed}.d^{-1}]$	 $4.2.10^{-6}$ O^{c} $1.8.10^{-8}$ O^{c}

[a] Already defined in STP sub-module.

* Different parameter value possible on regional and continental scale.

***Table III-198** Parameter settings for regional and continental soils.*

Parameter	Symbol	Unit	Value
Area fraction of natural soil region (27% of land area) continent	$F_{natural}$ *	[-]	0.267 0.135
Mixing depth of natural soil	$DEPTH_{natural}$	[m]	0.05
Area fraction of agricultural soil region (60% of land area) continent	F_{agric} *	[-]	0.594 0.30
Mixing depth of agricultural soil	$DEPTH_{agric}$	[m]	0.2
Area fraction of industrial/urban soil (10% of land area) region continent	F_{ind} *	[-]	0.099 0.05
Mixing depth of industrial/urban soil	$DEPTH_{ind}$	[m]	0.05
Fraction of rainwater infiltrating soil	$Finf_{soil}$	[-]	0.25
Fraction of rainwater run-off from soil	$Frunoff_{soil}$	[-]	0.25
Soil-erosion rate	EROSION	$[m.d^{-1}]$	$8.2.10^{-8}$

* Different parameter value possible on regional and continental scale.

***Table III-199** Mass-transfer coefficients for regional and continental scales.*

Parameter	Symbol	Unit	Value
Partial mass-transfer coefficient air side of air-soil interfaces	$kasl_{air}$	$[m.d^{-1}]$	90,5
Partial mass-transfer coefficient soil side of air-soil interface	$Kasl_{soil}$	$[m.d^{-1}]$	Equation 132
Partial mass-transfer coefficient air side of air-water interface	kaw_{air}	$[m.d^{-1}]$	Equation 139
Partial-mass transfer coefficient water side of air-water interface	kaw_{water}	$[m.d^{-1}]$	Equation 140
Partial mass-transfer coefficient water side sediment-water interface	kws_{water}	$[m.d^{-1}]$	0.24
Partial mass-transfer coefficient sediment side sediment-water interface	kws_{sed}	$[m.d^{-1}]$	$2.4.10^{-3}$

The regional distribution module is handled within this documentation as a 'black-box', only described by it's inputs and outputs. Several parameters, however, must be specified outside the SimpleBox calculation routines. Firstly, since the regional system is nested within the continental system, the values for area and population of the continental system must exclude the regional system.

In the following sections, calculations are given for the parameters that are specified in the TGD (and in the tables above) but are actually intermediate calculation results: residence times in air and water, and net sedimentation rate. These results are closed, to guard the internal consistency of the model.

Water in SimpleBox is treated as a bulk compartment. The last section shows the derivation of the dissolved concentration from the total concentration.

III.4.4.1 Area and population of the continental system

The area and population of the continental system are derived from the value for the total EU and the regional definition.

$$AREA(cont) = AREA(EU) - AREA(reg) \qquad (657)$$

Input			
AREA(EU)	area of EU	[m^2]	D
AREA(reg)	area of regional system	[m^2]	D
Output			
AREA(cont)	area of continental system	[m^2]	O^c

$$N(cont) = N(EU) - N(reg) \qquad (658)$$

Input			
N(EU)	number of inhabitants of EU	[eq]	D
N(reg)	number of inhabitants of region	[eq]	D
Output			
N(cont)	number of inhabitants of continental system	[eq]	O^c

III.4.4.2 Residence time in air

The residence time of air in the system is given by the area of the system and the wind speed.

$$TAU_{air} = \frac{\sqrt{AREA \cdot \frac{\pi}{4}}}{WINDSPEED} \qquad \textbf{(659)}$$

Input			
AREA	area of the system	[m^2]	D*
WINDSPEED	wind speed	[m.d^{-1}]	D
Output			
TAU_{air}	residence time of air	[d]	O*^{c}

III.4.4.3 Residence time in water

The total water flow through the system is caused by inflow from the larger spatial scale, wastewater production, run-off from soil, and direct rainfall into surface waters.

$$FLOW_{water} = Fflow_{out} \cdot FLOW_{water}(*) + WASTEW + RUNOFF + RAINDIRECT \qquad \textbf{(660)}$$

Input			
$FLOW_{water}$(*)	total water flow through system on larger spatial scale	[m^3.d^{-1}]	O*^{c}
$Fflow_{out}$	fraction of water flow from larger scale to system	[-]	D*
WASTEW	wastewater produced by inhabitants of system	[m^3.d^{-1}]	O*^{c}
RUNOFF	rainwater run-off from soil	[m^3.d^{-1}]	O*^{c}
RAINDIRECT	rainfall directly into surface water	[m^3.d^{-1}]	O*^{c}
Output			
$FLOW_{water}$	total water flow through system	[m^3.d^{-1}]	O*^{c}

The residence time of water in the system is given by the volume of the water compartment, divided by the total water flow through the system.

$$TAU_{water} = \frac{AREA \cdot F_{water} \cdot DEPTH_{water}}{FLOW_{water}} \qquad \textbf{(661)}$$

Input			
AREA	area of system	[m^2]	D*
F_{water}	area fraction of water	[-]	D*
$DEPTH_{water}$	water depth	[m]	D*
$FLOW_{water}$	total water flow through system	[m^3.d^{-1}]	O*^{c}
Output			
TAU_{water}	residence time of water	[d]	O*^{c}

Water flow through the system due to rainfall directly into surface water:

$$\boldsymbol{RAINDIRECT = RAINRATE \cdot AREA \cdot F_{water}} \qquad \mathbf{(662)}$$

Input			
RAINRATE	average daily precipitation	$[m.d^{-1}]$	D
AREA	area of system	$[m^2]$	D*
F_{water}	area fraction of water	[-]	D*
Output			
RAINDIRECT	rainfall directly into surface water	$[m^3.d^{-1}]$	O^{*c}

Rainwater run-off from soil:

$$\boldsymbol{RUNOFF = Frunoff_{soil} \cdot (F_{natural} + F_{agric} + F_{ind}) \cdot AREA \cdot RAINRATE} \qquad \mathbf{(663)}$$

Input			
$Frunoff_{soil}$	fraction of rainwater run-off from soil	[-]	D
$F_{natural}$	area fraction of natural soil	[-]	D*
F_{agric}	area fraction of agricultural soil	[-]	D*
F_{ind}	area fraction of industrial/urban soil	[-]	D*
AREA	area of system	$[m^2]$	D*
RAINRATE	average daily precipitation	$[m.d^{-1}]$	D
Output			
RUNOFF	rainwater run-off from soil	$[m^3.d^{-1}]$	O^{*c}

Wastewater produced by inhabitants of the system:

$$\boldsymbol{WASTEW = N \cdot Q_{stp}} \qquad \mathbf{(664)}$$

Input			
N	number of inhabitants of system	[eq]	D*
Q_{stp}	per-capita sewage flow	$[m^3.eq^{-1}.d^{-1}]$	D
Output			
WASTEW	wastewater produced by inhabitants of system	$[m^3.d^{-1}]$	O^{*c}

III.4.4.4 Net sedimentation rate in region

The suspended matter balance leads to the net sedimentation rate. Suspended matter enters the system through production, inflow from outside, effluent of sewage treatment and erosion of soil surfaces. Suspended matter leaves the system with the outflowing water.

$$NETsedrate =$$

$$\begin{aligned} &[\ SUSPPROD_{water} + SUSP_{water}(*) \cdot Fflow_{out} \cdot FLOW_{water}(*) + \\ &SUSP_{eff} \cdot EFFLUENT_{stp} + EROSION \cdot (F_{natural} + F_{agric} + F_{ind}) \cdot \\ &AREA \cdot Fsolid_{soil} \cdot RHOsolid - SUSP_{water} \cdot FLOW_{water}\ ] \\ &\cdot \frac{1}{Fsolid_{sed} \cdot RHOsolid} \cdot \frac{1}{AREA \cdot F_{water}} \end{aligned} \qquad (665)$$

Input			
$SUSPPROD_{water}$	(biogenic) production of suspended solids in water	$[kg_{dwt}.d^{-1}]$	D
$FLOW_{water}$	total water flow through system	$[m^3.d^{-1}]$	O^{*c}
$FLOW_{water}$ (*)	total water flow through system on larger spatial scale	$[m^3.d^{-1}]$	O^{*c}
$Fflow_{out}$	fraction of water flow from larger scale to system	[-]	D*
$SUSP_{water}$	suspended-solids concentration in water	$[kg_{dwt}.m^{-3}]$	D*
$SUSP_{water}$ (*)	suspended-solids concentration in water on larger scale	$[kg_{dwt}.m^{-3}]$	D*
$SUSP_{eff}$	suspended solids concentration in STP effluent	$[kg_{dwt}.m^{-3}]$	D
$EFFLUENT_{stp}$	effluent of STP	$[m^3.d^{-1}]$	O^{*c}
EROSION	soil-erosion rate	$[m.d^{-1}]$	D
$F_{natural}$	area fraction of natural soil	[-]	D*
F_{agric}	area fraction of agricultural soil	[-]	D*
F_{ind}	area fraction of industrial/urban soil	[-]	D*
F_{water}	area fraction of water	[-]	D*
AREA	area of system	$[m^2]$	D*
$Fsolid_{soil}$	fraction of solids in soil	$[kg.kg^{-1}]$	D
$Fsolid_{sed}$	fraction of solids in sediment	$[kg.kg^{-1}]$	D
RHOsolid	bulk density of solids	$[kg.m^{-3}]$	D
Output			
NETsedrate	net sedimentation rate	$[m.d^{-1}]$	O^{*c}

III.4.4.5 Regional and continental effluent discharges

The effluent discharge from regional and continental STPs depends on the fraction connected to treatment plants.

$$EFFLUENT_{stp} = N \cdot Q_{stp} \cdot Fconnect_{stp} \tag{666}$$

Input			
N	number of inhabitants of system	[eq]	D*
Q_{stp}	per-capita sewage flow	$[m^3.eq^{-1}.d^{-1}]$	D
$Fconnect_{stp}$	fraction connected to sewer systems	[-]	D
Output			
$EFFLUENT_{stp}$	effluent of STP	$[m^3.d^{-1}]$	$O*^c$

III.4.4.6 Calculation of the dissolved concentration in surface water

In SimpleBox, water is treated as a bulk compartment, including biota and suspended matter. The model calculations therefore yield a total concentration in surface water. In subsequent calculations, and in risk characterisation, the dissolved concentration is required. Therefore, the total concentration is converted as follows. The bioconcentration factor for aquatic biota (BCF_{biota}) used in this equation to calculate the distribution over different phases is calculated from Equation (162/163). This parameter is closed and should be distinguished from BCF_{fish} since measured BCF data for fish cannot be assumed representative for all aquatic biota. It should be noted that when a *Kow* value is not entered (e.g. for a metal), BCF_{biota} is set to zero. If sorption to aquatic biota is relevant for the dissolved concentration in surface water, the *Kp* for suspended matter can be adjusted manually to account for this process.

$$PECreg_{water} = \frac{PECreg_{water,tot}}{1 + Kp_{susp} \cdot SUSP_{water} + BCF_{biota} \cdot BIOTA_{water}} \tag{667}$$

Input			
$PECreg_{water,tot}$	regional concentration in total surface water	$[kg_c.m^{-3}]$	O
Kp_{susp}	solids-water partition coefficient of suspended matter	$[m^3.kg_{solids}^{-1}]$	O
$SUSP_{water}$	concentration of suspended matter in water of region	$[kg_{dwt}.m^{-3}]$	D
BCF_{biota}	BCF for aquatic biota in regional/continental model	$[m^3.kg_{wwt}^{-1}]$	O^c
$BIOTA_{water}$	concentration of aquatic biota in regional system	$[kg_{wwt}.m^{-3}]$	D
Output			
$PECreg_{water}$	regional PEC in surface water	$[kg_c.m^{-3}]$	O

III.4.4.7 Calculation of porewater concentration in agricultural soil

The concentration in porewater is derived from the total concentration by using the soil-water partition coefficient and the bulk density of the soil. The porewater concentration is used to estimate concentrations in plants and drinking water for indirect human exposure.

$$\boldsymbol{PECreg_{agric,porew} = \frac{PECreg_{agric,porew} \cdot RHO_{soil}}{K_{soil\text{-}water}}} \qquad \textbf{(668)}$$

Input			
$PECreg_{agric}$	regional PEC in agricultural soil (total)	$[kg_c.kg_{wwt}^{-1}]$	O
RHO_{soil}	wet bulk density of soil	$[kg_{wwt}.m^{-3}]$	O^c
$K_{soil\text{-}water}$	soil-water partition coefficient	$[m^3.m^{-3}]$	O^c
Output			
$PECreg_{agric,porew}$	regional PEC in porewater of agricultural soil	$[kg_c.m^{-3}]$	O

III.4.4.8 Mass transfer at air-soil and air-water interface on regional and continental scale

Soil–air interface

A substance-dependent soil-side partial mass transfer coefficient (PMTC) at the soil-air interface $kasl_{soil}$ (m.d^{-1}) is deduced from the exponential concentration profile in soil:

$$kasl_{soil} = \left(Veff_{soil} + \frac{Deff_{soil}}{d_p} \right) \qquad \textbf{(669)}$$

In soil, processes of downward advection (pore water + small particles), diffusion (air, water, solids), and degradation take place simultaneously. These processes are included in Simplebox 3.0 (Hollander *et al.*, 2003). The result is an exponential decrease of the concentration with depth (C_z), characterised by a substance-dependent penetration depth (d_p)

$$C_z = C_0 \cdot e^{-z/d_p}; \qquad d_p = \frac{Veff_{soil} + \sqrt{Veff_{soil}^{\;2} + Deff_{soil} \cdot k\deg_{soil}}}{2 \cdot k\deg_{soil}} \qquad \textbf{(670)}$$

in which:

$$Veff_{soil} = FRw.soil \frac{RAINRATE \cdot F\inf_{soil}}{Fwater_{soil}} + FRs.soil.\frac{SOLIDadv.soil}{Fsolid_{soil}} \qquad \textbf{(671)}$$

$$Deff_{soil} = FRa.soil \frac{DIFFgas \cdot Fair_{soil}^{\;1.5}}{Fair_{soil}} + FRw.soil.\frac{DIFFwater \cdot Fwater_{soil}^{\;1.5}}{Fwater_{soil}} + FRs.soil \cdot \frac{SOLIDdiff.soil}{Fsolid_{soil}} \qquad \textbf{(672)}$$

$$FRw.soil = \frac{Fwater_{soil}}{Fair_{soil} \cdot K_h^{'} + Fwater_{soil} + Fsolid_{soil} \cdot K_p^{'}} \qquad \textbf{(673)}$$

$$FRs.soil = \frac{Fsolid_{soil}}{Fair_{soil} \cdot K_h^{'} / K_p^{'} + Fwater_{soil} / K_p^{'} + Fsolid_{soil}} \qquad \textbf{(674)}$$

$$FRa.soil = 1 - FRw.soil - FRs.soil \qquad \textbf{(675)}$$

Input

$kdeg_{soil}$	rate constant for degradation in bulk soil	$[d^{-1}]$	O
RAINRATE	average daily rate of precipitation	$[m.d^{-1}]$	D
$Finf_{soil}$	fraction of precipitation that penetrates into the soil.	[-]	D
d_p	substance-dependent penetration depth	[m]	O^c
$Veff_{soil}$	effective advection (with penetrating porewater)	$[m.d^{-1}]$	O^c
$Deff_{soil}$	effective diffusion coefficient	$[m^2.d^{-1}]$	O^c
FRa.soil	mass fractions of the substance in the air phases of the soil	[-]	O^c
FRw.soil	mass fractions of the substance in the water phases of the soil	[-]	O^c
FRs.soil	mass fractions of the substance in the solid phases of the soil	[-]	O^c
$Fair_{soil}$	volume fractions of air in the soil compartment	$[m_{air}^{3}.m_{soil}^{-3}]$	D
$Fwater_{soil}$	volume fractions of water in the soil compartment	$[m_{water}^{3}.m_{soil}^{-3}]$	D
$Fsolid_{soil}$	volume fractions of solids in the soil compartment	$[m_{solid}^{3}.m_{soil}^{-3}]$	D
Kh'	dimensionless part. coeff. between gas- and water phases of air	[-]	O^c
Kp'	dimensionless part. coeff. between pore water- and solid phases of soil	[-]	O^c
DIFFgas	molecular diffusivity of the substance in the gas phases	$[m^2.d^{-1}]$	O^c
DIFFwater	molecular diffusivity of the substance in the water phases	$[m^2.d^{-1}]$	O^c
SOLIDadv.soil	rate of advective downward transport of soil particles	$[m.d^{-1}]$	O^c
SOLIDdiff.soil	solid phase diffusion coefficient in the soil compartment	$[m^2.d^{-1}]$	O^c

Output

$kasl_{soil}$	Partial mass-transfer coefficient soil side of air-soil interface	$[m.d^{-1}]$	O

Water-air interface

The partial mass transfer coefficients (PMTC) of the air-water interface depend on the windspeed of the system and the molecular weight of the substance:

$$kaw_{air} = 0.01 \cdot (0.3 + 0.2 \cdot WINDSPEED) \cdot ((0.018/MOLW)^{(0{,}67 \cdot 0{,}5)} \quad \textbf{(676)}$$

$$kaw_{water} = 0.01 \cdot (0.0004 + 0.0004 \cdot WINDSPEED^2) \cdot (0.032/MOLW)^{(0{,}5 \cdot 0{,}5)} \quad \textbf{(677)}$$

Input

WINDSPEED	wind speed of system	$[m.d^{-1}]$	D
MOLW	molecular weight	$[kg_c.mol^{-1}]$	S

Output

kaw_{air}	Partial mass-transfer coefficient air side of air-water interface	$[m.d^{-1}]$	O
kaw_{water}	Partial-mass transfer coefficient water side of air-water interface	$[m.d^{-1}]$	O

III.4.5 Local environmental distribution

In this section, the calculation of local environmental concentrations (*PEClocal*) is presented. Dedicated models are used for the compartments air, surface water and soil. Concentrations in sediment and groundwater are derived from the concentrations in surface water and soil, respectively. It should be noted that these calculations are performed for each relevant application and each step of the life cycle.

Several intermediate results of the soil sub-module are closed, since these results are too strictly model-related to allow for changes by the user (e.g. the concentration after 10 years due to deposition only: $Cdep10_i$).

Input: local direct emissions			
$Elocal_{air}$	local direct emission rate to air during episode	$[kg_c.d^{-1}]$	
Temission	number of days per year that emission takes place	$[d.year^{-1}]$	
Input: indirect emissions via STP			
$Estp_{air}$	local indirect emission to air from STP during episode	$[kg_c.d^{-1}]$	
$Clocal_{eff}$	concentration of chemical in STP effluent	$[kg_c.m^{-3}]$	
C_{sludge}	concentration in dry sewage sludge	$[kg_c.kg_{dwt}^{-1}]$	
$EFFLUENTlocal_{stp}$	effluent discharge rate of local STP	$[m^3.d^{-1}]$	c
Input: chemical properties			
$Fass_{aer}$	fraction of chemical bound to aerosol	[-]	
$K_{air-water}$	air-water partition coefficient	$[m^3.m^{-3}]$	c
$K_{soil-water}$	soil-water partition coefficient	$[m^3.m^{-3}]$	c
$K_{susp-water}$	suspended matter-water partition coefficient	$[m^3.m^{-3}]$	c
Kp_{susp}	solids-water partition coefficient of suspended matter	$[m^3.kg^{-1}]$	
$kdeg_{soil}$	rate constant for degradation in soil	$[d^{-1}]$	
Input background concentrations			
$PECreg_{air}$	regional concentration in air	$[kg_c.m^{-3}]$	
$PECreg_{water}$	regional concentration in surface water	$[kg_c.m^{-3}]$	
$PECreg_{water,marine}$	regional concentration in marine surface water	$[kg_c.m^{-3}]$	
$PECreg_{natural}$	regional concentration in natural soil	$[kg_c.kg_{wwt}^{-1}]$	
Intermediate results 1: removal rate constants soil			
$k_{volat\ i}$	rate constant for volatilisation from soil *i*	$[d^{-1}]$	
$k_{leach\ i}$	rate constant for leaching from soil *i* $i \in \{soil,agric,grassland\}$	$[d^{-1}]$	
k_i	total rate constant for removal from topsoil *i*	$[d^{-1}]$	
Intermediate results 2			
$Clocal_{air}$	local concentration in air during emission episode	$[kg_c.m^{-3}]$	
$Clocal_{air,ann}$	annual average concentration in air, 100 m from point source	$[kg_c.m^{-3}]$	
DEPtotal	total deposition flux during emission episode	$[kg_c.m^{-2}.d^{-1}]$	
$DEPtotal_{ann}$	annual average total deposition flux	$[kg_c.m^{-2}.d^{-1}]$	
$Clocal_{water}$	local concentration in surface water during emission episode	$[kg_c.m^{-3}]$	
$Clocal_{water,ann}$	annual average local concentration in surface water	$[kg_c.m^{-3}]$	
$Clocal_{water,marine}$	local conc. in marine surface water during emission episode	$[kg_c.m^{-3}]$	
$Clocal_{water,ann,marine}$	annual average local concentration in marine surface water	$[kg_c.m^{-3}]$	
$Clocal_{soil}$	local concentration in agric. soil averaged over 30 days (to assess terrestrial ecosystem)	$[kg_c.kg_{wwt}^{-1}]$	
$Clocal_{agric}$	local concentration in agric. soil averaged over 180 days (to calculate concentration in crops)	$[kg_c.kg_{wwt}^{-1}]$	
$Clocal_{grassland}$	local concentration in grassland averaged over 180 days	$[kg_c.kg_{wwt}^{-1}]$	
$Fst\text{-}st_i$	fraction of steady-state situation achieved in soil *i* $i \in \{soil,agric,grassland\}$	[-]	c

Output

$PEClocal_{air,ann}$	annual average local PEC in air (total)	$[kg_c.m^{-3}]$
$PEClocal_{water}$	predicted environmental concentration during episode	$[kg_c.m^{-3}]$
$PEClocal_{water,ann}$	annual average local PEC in surface water (dissolved)	$[kg_c.m^{-3}]$
$PEClocal_{water,marine}$	predicted environmental conc. in marine water during episode	$[kg_c.m^{-3}]$
$PEClocal_{water,ann,marine}$	annual average local PEC in marine surface water (dissolved)	$[kg_c.m^{-3}]$
$PEClocal_{sed}$	predicted environmental concentration in sediment	$[kg_c.kg^{-1}]$
$PEClocal_{sed,marine}$	predicted environmental concentration in marine sediment	$[kg_c.kg^{-1}]$
$PEClocal_{soil}$	local PEC in agric. soil (total) averaged over 30 days	$[kg_c.kg^{-1}]$
`	(to assess terrestrial ecosystem)	
$PEClocal_{agric}$	local PEC in agric. soil (total) averaged over 180 days	$[kg_c.kg^{-1}]$
	(to calculate concentration in crops)	
$PEClocal_{grassland}$	local PEC in grassland (total) averaged over 180 days	$[kg_c.kg^{-1}]$
$PEClocal_{agric,porew}$	local PEC in pore water of agricultural soil	$[kg_c.m^{-3}]$
$PEClocal_{grassland,porew}$	local PEC in pore water of grassland	$[kg_c.m^{-3}]$
$PEClocal_{grw}$	local PEC in groundwater under agricultural soil	$[kg_c.m^{-3}]$

Table III-200 *Default settings of the local environmental fate models.*

Parameter	**Symbol**	**Unit**	**Value**
Air			
concentration in air at source strength 1 $kg.d^{-1}$	$Cstd_{air}$	$[kg_c.m^{-3}]$	$2.78.10^{-10}$
deposition flux of aerosol-bound chemical at 1 $kg.d^{-1}$	$DEPstd_{aer}$	$[kg_c.m^{-2}.d^{-1}]$	1.10^{-8}
deposition flux of gaseous compounds at 1 $kg.d^{-1}$ $^{10}\log HENRY < -2$ $-2 < {}^{10}\log HENRY < 2$ $^{10}\log HENRY > 2$	$DEPstd_{gas}$	$[kg_c.m^{-2}.d^{-1}]$	 5.10^{-10} 4.10^{-10} 3.10^{-10}
Surface water			
concentration of suspended matter in river water	$SUSP_{water}$	$[kg_{dwt}.m^{-3}]$	0.015 [a]
dilution factor after complete mixing Freshwater environment Marine environment	 DILUTION $DILUTION_{marine}$	 [-] [-]	 10 100[b]
Soil			
Partial mass transfer coefficient at air side of air-soil interface	$kasl_{air}$	$[m.d^{-1}]$	90,5 [a]
Partial mass-transfer coefficient at soil side of air-soil interface	$kasl_{soil}$	$[m.d^{-1}]$	Equation 130 [a]
Fraction of rainwater infiltrating in soil	$Finf_{soil}$	[-]	0.25 [a]
Rate of wet precipitation (700 mm/year)	RAINRATE	$[m.d^{-1}]$	$1.92.10^{-3}$ [a]

[a] Already defined in regional distribution sub-module.

[b] For discharges to a coastal zone, local dilution will be greater than in a freshwater river. First, initial dilution may occur if the density between the effluent and the saline receiving medium differs. The initial dilution factor is usually around 10. Further dilution due to currents can also be assumed, particularly if the point of release is subject to tidal influences. A dilution factor for discharges to a coastal zone of 100 may then be assumed, which seems to be representative for a realistic worst case. This dilution factor is related to a discharge volume of 2000 m^3/d.

III.4.5.1 Local concentration in air and deposition flux

The air compartment receives its input from direct emissions to air, and volatilisation from the sewage treatment plant. The concentration in air is used as input for indirect exposure of humans via inhalation. Deposition fluxes are used as input for the calculation of local concentrations in soil. Therefore, both deposition flux and concentration in air are calculated as annual average values. The Gaussian plume model OPS, as described by Van Jaarsveld (1990), is applied using the standard parameters given by Toet and de Leeuw (1992). The OPS results are used as the standard concentration and deposition flux at a source strength of 1 kg/d. The concentration of the chemical is calculated at 100 m distance from the point source and the STP, and the higher of these two is used.

$$Clocal_{air} = \max\left(Elocal_{air}, Estp_{air} \right) \cdot Cstd_{air} \qquad (678)$$

$$Clocal_{air,ann} = Clocal_{air} \cdot \frac{Temission}{365} \qquad (679)$$

Input			
$Elocal_{air}$	local direct emission rate to air during episode	$[kg_c.d^{-1}]$	O
$Estp_{air}$	local indirect emission to air from STP during episode	$[kg_c.d^{-1}]$	O
$Cstd_{air}$	concentration in air at source strength of 1 kg.d^{-1}	$[kg_c.m^{-3}]$	D
Temission	number of days per year that emission occurs	$[d.year^{-1}]$	O
Output			
$Clocal_{air}$	local concentration in air during episode, 100 m from source	$[kg_c.m^{-3}]$	O
$Clocal_{air,ann}$	annual average concentration in air, 100 m from source	$[kg_c.m^{-3}]$	O

The air concentration on the regional scale is used as the background concentration for the local scale, and is therefore, summed to the local concentration.

$$PEClocal_{air,ann} = Clocal_{air,ann} + PECregional_{air} \qquad (680)$$

Input			
$Clocal_{air,ann}$	annual average local concentration in air	$[kg_c.m^{-3}]$	O
$PECreg_{air}$	regional concentration in air	$[kg_c.m^{-3}]$	O
Output			
$PEClocal_{air,ann}$	annual average predicted environmental conc. in air	$[kg_c.m^{-3}]$	O

In calculating the deposition flux, the emissions from the two sources (direct and STP) are summed.

$$DEPtotal = \left(Elocal_{air} + Estp_{air} \right) \cdot \left(Fass_{aer} \cdot DEPstd_{aer} + (1 - Fass_{aer}) \cdot DEPstd_{gas} \right) \quad (681)$$

$$DEPtotal_{ann} = DEPtotal \cdot \frac{Temission}{365} \quad (682)$$

Input			
$Elocal_{air}$	local direct emission rate to air during emission episode	$[kg_c.d^{-1}]$	O
$Estp_{air}$	local indirect emission to air from STP during episode	$[kg_c.d^{-1}]$	O
$Fass_{aer}$	fraction of chemical bound to aerosol	[-]	O
$DEPstd_{aer}$	standard deposition flux of aerosol-bound compounds at source strength of 1 $kg.d^{-1}$	$[kg_c.m^{-2}.d^{-1}]$	D
$DEPstd_{gas}$	deposition flux of gaseous compounds as function of Henry's Law coefficient, at source strength of 1 $kg.d^{-1}$	$[kg_c.m^{-2}.d^{-1}]$	D
Temission	number of days per year that emission occurs	$[d.yr^{-1}]$	O
Output			
DEPtotal	total deposition flux during emission episode	$[kg_c.m^{-2}.d^{-1}]$	O
$DEPtotal_{ann}$	annual average total deposition flux	$[kg_c.m^{-2}.d^{-1}]$	O

III.4.5.2 Local concentration in surface water (freshwater and marine environment)

The effluent of the sewage treatment plant is discharged into surface water. Dilution in the receiving surface water and sorption to suspended solids are taken into account. The fixed dilution factor represents the dilution at the point of complete mixing of effluent and receiving water. EUSES will perform a check whether the concentration exceeds the water solubility. If this is the case, the results of this module should be studied in more detail on a case-by-case basis. The concentration during an emission episode is calculated for exposure of aquatic organisms. An annual average concentration is calculated for assessing indirect human exposure and secondary poisoning.

For estuaries, which are influenced by currents and tidal movements, it is assumed as a first approach that either the inland or the marine risk assessment covers them. Thus, no specific assessment is proposed. Then, the local concentrations in seawater can be obtained with the same equations as presented for the freshwater approach.

$$Clocal_{water} = \frac{Clocal_{eff}}{(1 + Kp_{susp} \cdot SUSP_{water}) \cdot DILUTION} \quad (683)$$

$$Clocal_{water,marine} = \frac{Clocal_{eff}}{(1 + Kp_{susp} \cdot SUSP_{water}) \cdot DILUTION_{marine}} \quad (684)$$

$$Clocal_{water,ann} = Clocal_{water} \cdot \frac{Temission}{365} \quad (685)$$

$$Clocal_{water,ann,marine} = Clocal_{water,marine} \cdot \frac{Temission}{365} \quad (686)$$

Input			
$Clocal_{eff}$	concentration of chemical in the STP effluent	$[kg_c.m^{-3}]$	O
Kp_{susp}	solids-water partition coefficient of suspended matter	$[m^3.kg^{-1}]$	O
$SUSP_{water}$	concentration of suspended matter in river water	$[kg_{dwt}.m^{-3}]$	D
DILUTION	dilution factor (freshwater environment)	[-]	D/O^c
$DILUTION_{marine}$	dilution factor (marine environment)	[-]	D
Temission	number of days per year that emission occurs	$[d.yr^{-1}]$	O
Output			
$Clocal_{water}$	local concentration in surface water during emission episode	$[kg_c.m^{-3}]$	O
$Clocal_{water,ann}$	annual average local concentration in surface water	$[kg_c.m^{-3}]$	O
$Clocal_{water,marine}$	local conc. in marine surface water during emission episode	$[kg_c.m^{-3}]$	O
$Clocal_{water,ann,marine}$	annual average local concentration in marine surface water	$[kg_c.m^{-3}]$	O

When a more site-specific assessment is appropriate, account should be taken of the fluctuating flow-rates of typical receiving waters. The low-flow rate (or 10th-percentile) should always be used. Where only average flows are available, the flow for dilution purposes should be estimated as one third of this average. The actual dilution factor after complete mixing can be calculated from the flow rate of the river and the effluent discharge rate. This approach should be used for rivers only and not for estuaries or lakes. A default dilution factor for discharges to a coastal zone of 100 is assumed to be representative for a realistic worst case. In case of site-specific assessment the dilution factor applied for the local concentration in surface water should not be greater than 1000.

$$DILUTION = \frac{EFFLUENTlocal_{stp} + FLOW}{EFFLUENTlocal_{stp}} \quad (687)$$

Input			
$EFFLUENTlocal_{stp}$	effluent discharge rate of local STP	$[m^3.d^{-1}]$	O^c
FLOW	flow rate of the river	$[m^3.d^{-1}]$	D
Output			
DILUTION	dilution factor (freshwater environment)	[-]	D/O^c

The concentration on the regional scale is used as background concentration for the local scale. Therefore, these concentrations are summed.

$$PEClocal_{water} = Clocal_{water} + PECreg_{water} \tag{688}$$

$$PEClocal_{water,marine} = Clocal_{water,marine} + PECreg_{water,marine} \tag{689}$$

$$PEClocal_{water,ann} = Clocal_{water,ann} + PECreg_{water} \tag{690}$$

$$PEClocal_{water,ann,marine} = Clocal_{water,ann,marine} + PECreg_{water,marine} \tag{691}$$

Input			
$Clocal_{water}$	local concentration in surface water during episode	$[kg_c.m^{-3}]$	O
$Clocal_{water,ann}$	annual average concentration in surface water	$[kg_c.m^{-3}]$	O
$PECreg_{water}$	regional concentration in surface water	$[kg_c.m^{-3}]$	O
$Clocal_{water,marine}$	local conc. in marine water during emission episode	$[kg_c.m^{-3}]$	O
$Clocal_{water,ann,marine}$	annual average local concentration in marine surface water	$[kg_c.m^{-3}]$	O
$PECreg_{water,marine}$	regional concentration in marine water	$[kg_c.m^{-3}]$	O
Output			
$PEClocal_{water}$	predicted environmental concentration during episode	$[kg_c.m^{-3}]$	O
$PEClocal_{water,ann}$	annual average local PEC in surface water	$[kg_c.m^{-3}]$	O
$PEClocal_{water,marine}$	predicted environmental conc. in marine water during episode	$[kg_c.m^{-3}]$	O
$PEClocal_{water,ann,marine}$	annual average local PEC in marine water	$[kg_c.m^{-3}]$	O

III.4.5.3 Local concentration in sediment (freshwater and marine environment)

The concentration in freshly deposited sediment is taken as the PEC for sediment and the properties of suspended matter are therefore used. The concentration in bulk sediment is derived from the corresponding water-body concentration, assuming a thermodynamic partition equilibrium (see also Di Toro *et al.*, 1991). The local concentration in marine sediment can be obtained with the same approach as presented for freshwater sediment.

$$PEClocal_{sed} = \frac{K_{susp\text{-}water}}{RHO_{susp}} \cdot PEClocal_{water} \tag{692}$$

$$PEClocal_{sed,marine} = \frac{K_{susp\text{-}water}}{RHO_{susp}} \cdot PEClocal_{water,marine} \tag{693}$$

Input			
$PEClocal_{water}$	predicted environmental conc. in surface water during episode	$[kg_c.m^{-3}]$	O
$PEClocal_{water,marine}$	predicted environmental conc. in marine water during episode	$[kg_c.m^{-3}]$	O
$K_{susp-water}$	suspended matter-water partition coefficient	$[m^3.m^{-3}]$	O^c
RHO_{susp}	bulk density of suspended matter	$[kg_{wwt}.m^{-3}]$	O^c
Output			
$PEClocal_{sed}$	predicted environmental concentration in sediment	$[kg_c.kg_{wwt}^{-1}]$	O
$PEClocal_{sed,marine}$	predicted environmental concentration in marine sediment	$[kg_c.kg_{wwt}^{-1}]$	O

III.4.5.4 Local concentration in soil

Concentrations in soil are used as exposure concentrations for terrestrial organisms and for indirect exposure of humans (through crops, meat and dairy products). The topsoil layer is modelled as a single compartment, receiving input through application of sludge dressing and continuous airborne deposition, and with output via leaching, volatilisation and biodegradation. As the concentration is not constant during the year, the exposure concentration is averaged over a certain time period. Ten years of accumulation is accounted for. Three different PECs are calculated in soil, for different end-points (Table III-201).

Table III-201 *Characteristics of soil and soil-use for the three different endpoints.*

Type of soil	**Depth of soil compartment [m]**	**Averaging time [days]**	**Rate of sludge application [$kg_{dwt}.m^{-2}.year^{-1}$]**	**End-point**
	$DEPTH_i$	T_i	$APPLsludge_i$	
Agricult. soil i = soil	0.20	30	0.5	terrestrial ecosystem
Agricult. soil i = agric	0.20 [a]	180	0.5	crops for human consumption and predators
Grassland i = grassland	0.10	180	0.1	grass for cattle

[a] Already defined in regional distribution sub-module

Derivation of the removal-rate constant

For removal from the topsoil, the following processes are quantified:

- biodegradation in soil;
- volatilisation of substance from soil;
- leaching to deeper soil layers.

The diffusive transfer from soil to air is estimated using the classical two-film resistance model. Given a substance-independent air-side partial mass transfer coefficient, $kasl_{air}$, the soil-referenced overall mass transfer coefficient, used for calculating the rate constant for volatilization, $k_{volat\ i}$, becomes:

$$\frac{1}{k_{volat\ i}} = \left(\frac{1}{kasl_{air} \cdot K_{air\text{-}water} / K_{soil-water}} + \frac{1}{kasl_{soil}} \right) \cdot DEPTH_i \qquad \textbf{(694)}$$

in which $K_{air\text{-}soil}$, $K_{air\text{-}water}$ and $K_{soil\text{-}water}$ are the dimensionless equilibrium constants between bulk air and bulk soil, bulk air and bulk water, and between bulk soil and bulk water, respectively, and *DEPTHi* (m) is the mixing depth of the soil compartment.

Input			
$kasl_{air}$	partial mass-transfer coeff. at air side of air-soil interface	$[m.d^{-1}]$	D
$kasl_{soil}$	partial mass-transfer coeff. at soil side of air-soil interface	$[m.d^{-1}]$	O
$K_{air-water}$	air-water partition coefficient	$[m^3.m^{-3}]$	O^c
$K_{soil-water}$	soil-water partition coefficient	$[m^3.m^{-3}]$	O^c
$DEPTH_i$	mixing depth of soil type *i*	[m]	D
Output			
$k_{volat\ i}$	rate constant for volatilisation from soil *i*	$[d^{-1}]$	O

A first-order rate constant for leaching can be calculated from the amount of rain flushing the liquid phase of the soil compartment.

$$k_{leach\ i} = \frac{Finf_{soil} \cdot RAINRATE}{K_{soil-water} \cdot DEPTH_i} \qquad (695)$$

Input			
$Finf_{soil}$	fraction of rainwater that infiltrates into soil	[-]	D
RAINRATE	rate of wet precipitation	$[m.d^{-1}]$	D
$K_{soil-water}$	soil-water partition coefficient	$[m^3.m^{-3}]$	O^c
$DEPTH_i$	mixing depth of soil type *i*	[m]	D
Output			
$k_{leach\ i}$	rate constant for leaching from soil *i*	$[d^{-1}]$	O

The overall removal-rate constant is given by the sum of all relevant-removal rate constants.

$$k_i = k_{volat\ i} + k_{leach\ i} + kdeg_{soil} \qquad (696)$$

Input			
$k_{volat\ i}$	rate constant for volatilisation from soil *i*	$[d^{-1}]$	O
$k_{leach\ i}$	rate constant for leaching from topsoil *i*	$[d^{-1}]$	O
$kdeg_{soil}$	rate constant for degradation in soil	$[d^{-1}]$	O
Output			
k_i	rate constant for removal from topsoil *i*	$[d^{-1}]$	O

Referencing deposition flux to kg soil

To simplify the calculations, the airborne deposition flux (Section III.4.5.1) is referenced to kg substance per kg of soil per day. The total deposition flux is converted as follows:

$$D_{air\ i} = \frac{DEPtotal_{ann}}{DEPTH_i \cdot RHO_{soil}} \qquad (697)$$

Input			
$DEPtotal_{ann}$	annual average total deposition flux	$[kg_c.m^{-2}.d^{-1}]$	O
$DEPTH_i$	mixing depth of soil type *i*	[m]	D
RHO_{soil}	bulk density of soil	$[kg_{wwt}.m^{-3}]$	O^c
Output			
$D_{air\ i}$	airborne deposition flux per kg of soil *i*	$[kg_c.kg_{wwt}^{-1}.d^{-1}]$	O^c

Initial concentration after 10 years of sludge application

To take accumulation in soil into account, sludge application is assessed for 10 consecutive years. The PEC in soil is the concentration in the 10th year, averaged over a time period *T*. As a first step, the initial concentration in this year needs to be derived. The contributions of deposition and sludge applications are considered separately. The concentration due to 10 years of continuous deposition only is given by:

$$Cdep10_i = \frac{D_{air\ i}}{k_i} - \frac{D_{air\ i}}{k_i} \cdot e^{-365 \cdot 10 \cdot k_i} \qquad (698)$$

Input			
$D_{air\ i}$	airborne deposition flux per kg of soil *i*	$[kg_c.kg_{wwt}^{-1}.d^{-1}]$	O
k_i	rate constant for removal from top-soil *i*	$[d^{-1}]$	O
Output			
$Cdep10_i$	concentration in soil *i* due to deposition in 10th year at t=0	$[kg_c.kg_{wwt}^{-1}]$	O^c

Sludge application is not a continuous process, but is assumed to take place once a year at the beginning of each year. The concentration just after the first year of sludge application is given by:

$$Csludge1_i = \frac{C_{sludge} \cdot APPLsludge_i}{DEPTH_i \cdot RHO_{soil}} \qquad (699)$$

Input			
C_{sludge}	concentration in dry sewage sludge	$[kg_c.kg_{dwt}^{-1}]$	O
$APPLsludge_i$	dry sludge application rate on soil *i*	$[kg_{dwt}.m^{-2}.yr^{-1}]$	D
$DEPTH_i$	mixing depth of soil type *i*	[m]	D
RHO_{soil}	bulk density of soil	$[kg_{wwt}.m^{-3}]$	O^c
Output			
$Csludge1_i$	concentration in soil due to sludge in first year at t=0	$[kg_c.kg_{wwt}^{-1}]$	O^c

At the end of each year, a fraction *Facc* of the initial concentration remains in the topsoil layer. Using this fraction, the initial concentration after 10 applications of sludge can be assessed.

$$Facc_i = e^{-365 k_i} \tag{700}$$

$$Csludge10_i = Csludge1_i \cdot \left[1 + \sum_{n=1}^{9} Facc_i^{\,n} \right] \tag{701}$$

Input			
k_i	rate constant for removal from top soil *i*	$[d^{-1}]$	O
$Facc_i$	fraction accumulating in one year in soil *i*	[-]	O^c
$Csludge1_i$	concentration in soil *i* due to sludge in first year at t=0	$[kg_c.kg_{wwt}^{-1}]$	O^c
Output			
$Csludge10_i$	concentration in soil *i* due to sludge in 10th year at t=0	$[kg_c.kg_{wwt}^{-1}]$	O^c

The sum of the concentrations due to deposition and to sludge is the initial concentration in year 10.

$$Clocal10_i = Cdep10_i + Csludge10_i \tag{702}$$

Input			
$Csludge10_i$	concentration in soil *i* due to sludge in 10th year at t=0	$[kg_c.kg_{wwt}^{-1}]$	O^c
$Cdep10_i$	concentration in soil *i* due to deposition in 10th year at t=0	$[kg_c.kg_{wwt}^{-1}]$	O^c
Output			
$Clocal10_i$	initial concentration in soil *i* (in 10th year at t=0)	$[kg_c.kg_{wwt}^{-1}]$	O^c

Local concentration in soil

The fate of the chemical in soil is modelled with a one-compartment model with a continuous input from airborne deposition and continuous elimination from the topsoil layer. The initial condition is given by $Clocal10_i$. The differential equation describing the one-compartment model can be solved analytically to give the concentration in soil as a function of time. The exposure concentration in soil was defined as the average concentration over a certain time period *T*, and is thus defined by the integral of the concentration in soil *i* from 0 to *T* days:

$$Clocal_i = \frac{1}{T_i} \cdot \int_0^{T_i} Clocal_i(t)\, dt \tag{703}$$

The analytical solution of this integral is then given by:

$$Clocal_i = \frac{D_{air\,i}}{k_i} + \frac{1}{k_i\,T_i}\left[Clocal\,10_i - \frac{D_{air\,i}}{k_i} \right] \cdot \left[1 - e^{-k_i T_i}\right] \tag{704}$$

Input			
$D_{air\,i}$	airborne deposition flux per kg of soil *i*	$[kg_c.kg_{wwt}^{-1}.d^{-1}]$	O^c
T_i	averaging time for soil *i*	[d]	D
k_i	rate constant for removal from topsoil *i*	$[d^{-1}]$	O
$Clocal10_i$	initial concentration in soil *i* (in 10th year at t=0)	$[kg_c.kg_{wwt}^{-1}]$	O^c
Output			
$Clocal_i$	average concentration in soil *i* over *T* days	$[kg_c.kg_{wwt}^{-1}]$	O

The concentration on the regional scale is used as the background concentration for the local scale. For this purpose, the concentration in natural soil is used (input through deposition only), for otherwise sludge application would be taken into account twice.

$$PEClocal_i = Clocal_i + PECreg_{natural} \tag{705}$$

Input			
$Clocal_i$	local concentration in soil *i*	$[kg_c.kg_{wwt}^{-1}]$	O
$PECreg_{natural}$	regional concentration in natural soil	$[kg_c.kg_{wwt}^{-1}]$	O
Output			
$PEClocal_i$	predicted environmental concentration in soil *i*	$[kg_c.kg_{wwt}^{-1}]$	O

Local concentration in pore water of soil

The concentration in the pore water of soil is calculated by applying the soil-water partition coefficient.

$$PEClocal_{i,porew} = \frac{PEClocal_i \cdot RHO_{soil}}{K_{soil-water}} \tag{706}$$

Input			
$PEClocal_i$	predicted environmental concentration in soil *i*	$[kg_c.kg_{wwt}^{-1}]$	O
$K_{soil-water}$	soil-water partition coefficient	$[m^3.m^{-3}]$	O^c
RHO_{soil}	bulk density of wet soil	$[kg_{wwt}.m^{-3}]$	O^c
Output			
$PEClocal_{i,porew}$	predicted environmental conc. in pore water of soil *i*	$[kg_c.m^{-3}]$	O

Persistence of the substance in soil

Ten consecutive years of accumulation may not be sufficient for some substances to reach a steady-state situation. These substance may accumulate for hundreds of years. To indicate the potential persistence in soil, the fraction of the steady-state concentration is calculated.

$$Fst-st_i = \frac{Clocal10_i}{Cinf_i} \tag{707}$$

Input			
$Clocal10_i$	initial concentration in soil *i* after 10 years	$[kg_c.kg_{wwt}^{-1}]$	O^c
$Cinf_i$	initial concentration in soil *i* in steady-state situation	$[kg_c.kg_{wwt}^{-1}]$	O^c
Output			
$Fst\text{-}st_i$	fraction of steady-state situation achieved in soil *i*	[-]	O^c

The initial concentration in the steady-state year is given by:

$$C\,inf_i = \frac{D_{air\,i}}{k_i} + Csludge1_i \cdot \frac{1}{1-Facc_i} \tag{708}$$

Input			
$D_{air\,i}$	airborne deposition flux per kg of soil *i*	$[kg_c.kg_{wwt}^{-1}.d^{-1}]$	O^c
k_i	rate constant for removal from topsoil *i*	$[d^{-1}]$	O
$Facc_i$	fraction accumulating in soil *i* in one year	[-]	O^c
$Csludge1_i$	concentration in soil *i* due to sludge in first year at t=0	$[kg_c.kg_{wwt}^{-1}]$	O^c
Output			
$Cinf_i$	initial concentration in soil *i* in steady-state situation	$[kg_c.kg_{wwt}^{-1}]$	O^c

III.4.5.5 Calculation of concentration in groundwater

The concentration in groundwater is calculated for indirect exposure of humans via drinking water. As an indication for potential groundwater levels, the concentration in pore water is taken after 10 years of sludge application to agricultural soil, averaged over 180 days. Transformation and dilution in deeper soil layers are not accounted for.

$$PEClocal_{grw} = PEClocal_{agric,porew} \tag{709}$$

Input			
$PEClocal_{agric,porew}$	predicted environmental conc. in pore water of agric. soil	$[kg_c.m^{-3}]$	O
Output			
$PEClocal_{grw}$	predicted environmental conc. in groundwater	$[kg_c.m^{-3}]$	O

III.5 EXPOSURE MODULE

In the exposure module, exposure levels for humans and predating birds and mammals are estimated. This module is divided into four specific sub-modules, which will be handled separately:

- Secondary poisoning.
- Indirect human exposure.
- Consumer exposure.
- Workplace exposure.

III.5.1 Secondary poisoning

For the assessment of secondary poisoning, three example food chains are modelled:

1. water (freshwater and marine environment)→fish→predator
2. water (marine environment)→fish→predator→toppredator
3. soil→worm→predator.

Exposure levels are calculated, assuming a scenario whereby 50% of the food is sourced from the local environment and 50% from the regional environment.

Input: chemical properties			
Kow	octanol-water partition coefficient	[-]	
Input: environmental properties			
RHO$_{soil}$	bulk density of soil	[kg$_{wwt}$.m^{-3}]	c
CONV$_{soil}$	conversion factor for soil concentrations: wwt to dwt	[kg$_{wwt}$.kg$_{dwt}^{-1}$]	c
PEClocal$_{water,ann}$	annual average local PEC in surface water (dissolved)	[kg$_{c}$.m^{-3}]	
PEClocal$_{water,ann,marine}$	annual average local PEC in marine surface water (dissolved)	[kg$_{c}$.m^{-3}]	
PEClocal$_{agric}$	local PEC in agricultural soil	[kg$_{c}$. kg$_{wwt}^{-1}$]	
PEClocal$_{agric,porew}$	local PEC in pore water of agricultural soil	[kg$_{c}$.m^{-3}]	
PECreg$_{water}$	regional PEC in surface water (dissolved)	[kg$_{c}$.m^{-3}]	
PECreg$_{water,marine}$	regional PEC in marine surface water (dissolved)	[kg$_{c}$.m^{-3}]	
PECreg$_{agric}$	regional PEC in agricultural soil	[kg$_{c}$.kg$_{wwt}^{-1}$]	
PECreg$_{agric,porew}$	regional PEC in pore water of agricultural soil	[kg$_{c}$.m^{-3}]	
Intermediate results			
BCF$_{worm}$	bioconcentration factor for earthworms	[kg$_{soil\ wwt}$.kg$_{worm\ wwt}^{-1}$]	
BCF$_{fish}$	bioconcentration factor for fish	[m^{3}.kg$_{wwt}^{-1}$]	
Output			
BCF$_{fish}$	bioconcentration factor for fish	[m^{3}.kg$_{wwt}^{-1}$]	
PEC$_{oral,fish}$	concentration in fish from surface water for predators	[kg$_{c}$.kg$_{wwt}^{-1}$]	
PEC$_{oral,fish,marine}$	concentration in fish from marine surface water for predators	[kg$_{c}$.kg$_{wwt}^{-1}$]	
PEC$_{oral,fish\ predator,marine}$	concentration in fish-eating predator for marine toppredators	[kg$_{c}$.kg$_{wwt}^{-1}$]	
PEC$_{oral,worm}$	concentration in earthworms from agricultural soil	[kg$_{c}$.kg$_{wwt}^{-1}$]	

III.5.1.1 Bioconcentration factor for fish

The methods that estimate a BCF for fish from log *Kow* are widely used and, in general, the most reliable. The following combination of QSARs is advised in Chapter 4 of the TGD. For substances with a log *Kow*, from 1 to 6, the relation by Veith *et al.* (1979) is used, while for substances in the log *Kow* range between 6 and 10 a parabolic equation is applied. Domain of physico-chemical properties: log *Kow* 1 to 10 (outside this range the minimum or maximum *Kow* is used), molecular weight less than 700 g/mol. For chemicals with a molecular weight of more than 700 g/mol, the BCF tends to decrease but in lack of experimental data, the QSAR can be used as an initial worst-case estimate.

if log *Kow* ≤ 6 then:

$$\log BCF_{fish} = 0.85 \cdot \log Kow - 0.70 - 3 \qquad \textbf{(710)}$$

if log *Kow* > 6 then:

$$\log BCF_{fish} = -0.20 \cdot (\log Kow)^2 + 2.74 \cdot \log Kow - 4.72 - 3 \qquad \textbf{(711)}$$

Input			
Kow	octanol-water partition coefficient	$[m^3.m^{-3}]$	S
Output			
BCF_{fish}	bioconcentration factor for fish	$[m^3.kg_{wwt}^{-1}]$	O

III.5.1.2 Exposure concentration for predators in freshwater and marine environment

The biomagnification factor (BMF) is defined as the relative concentration in a predatory animal compared to the concentration in its prey (BMF = Cpredator/Cprey). The BMF should ideally be based on measured data. However, the availability of such data is at present very limited and therefore, the default values given in Table III-202 should be used. By establishing these factors it is assumed that a relationship exists between the BMF, the BCF and the log Kow. If a BCF for fish is available, it is possible to use that as a trigger instead of log Kow. The BCF triggers recommended are less conservative than the log Kow triggers because they more realistically take the potential for metabolism in biota (i.e. fish) into account. Due to this increased relevance, the use of a measured BCF would take precedence over a trigger based on log Kow.

Table III-202 *Default BMF values for organic substances.*

Log Kow $[m^3.m^{-3}]$	**BCF (fish)** $[m^3.kg_{wwt}^{-1}]$	**BMF_1** [-]	**BMF_2** [-]
< 4.5	< 2	1	1
4.5 - <5	2 – 5	2	2
5 - 8	> 5	10	10
>8 – 9	5 – 2	3	3
> 9	< 2	1	1

Input			
Kow	octanol-water partition coefficient	$[m^3.m^{-3}]$	P
BCF_{fish}	bioconcentration factor for fish	$[m^3.kg_{wwt}^{-1}]$	P
Output			
BMF	biomagnification factor in fish/predator	[-]	O

The exposure level for the first tier of organisms, the fish-eating predators, in freshwater and marine water ($PEC_{oral,fish}$) is calculated from the average of the local and regional PEC for surface water, the measured or estimated BCF for fish and the biomagnification factor (BMF_1).

$$PEC_{oral,\,fish} = 0.5 \cdot (PEClocal_{water,ann} + PECreg_{water}) \cdot BCF_{fish} \cdot BMF_1 \qquad (712)$$

$$PEC_{oral,\,fish,marine} = 0.5 \cdot (PEClocal_{water,ann,marine} + PECreg_{water,marine}) \cdot BCF_{fish} \cdot BMF_1 \qquad (713)$$

Input			
BCF_{fish}	bioconcentration factor for fish	$[m^3.kg_{wwt}^{-1}]$	O
$PEClocal_{water,ann}$	annual average local PEC in surface water (dissolved)	$[kg_c.m^{-3}]$	O
$PECreg_{water}$	regional PEC in surface water (dissolved)	$[kg_c.m^{-3}]$	O
$PEClocal_{water,ann,marine}$	annual average local PEC in marine surface water (dissolved)	$[kg_c.m^{-3}]$	O
$PECreg_{water,marine}$	regional PEC in marine surface water (dissolved)	$[kg_c.m^{-3}]$	O
BMF_1	biomagnification factor in fish	[-]	P
Output			
$PEC_{oral,fish}$	conc. in fish for secondary poisoning in freshwater environment	$[kg_c.kg_{wwt}^{-1}]$	O
$PEC_{oral,fish,marine}$	conc. in fish for secondary poisoning in marine environment	$[kg_c.kg_{wwt}^{-1}]$	O

The food chain of the marine environment is, besides a fish-eating predator, also modelled with a toppredator. Toppredators pray on organisms that are in direct contact with the marine aqueous phase and receive the substances from this source (fish-eating predator). For the second tier of organisms, the top-predators, it can be assumed that they obtain their prey mainly from the larger-scale regional marine environment that is to a lesser extent influenced by point source discharges. However, since it cannot be ruled out that certain top-predators prey on organisms that receive their food from relatively small areas it is proposed to assume, as a realistic worst case, a 90/10 ratio between regional and local food intake.

$$PEC_{oral,\,fish\ predator,marine} = (0.1 \cdot PEClocal_{water,ann,marine} + 0.9 \cdot PECreg_{water,marine}) \cdot BCF_{fish} \cdot BMF_1 \cdot BMF_2 \qquad (714)$$

Input			
$PEClocal_{water,ann,marine}$	annual average local PEC in marine surface water (dissolved)	$[kg_c.m^{-3}]$	O
$PECreg_{water,marine}$	regional PEC in marine surface water (dissolved)	$[kg_c.m^{-3}]$	O
BCF_{fish}	bioconcentration factor for fish	$[m^3.kg_{wwt}^{-1}]$	O
BMF_1	biomagnification factor in fish	[-]	O
BMF_2	biomagnification factor in predator	[-]	O
Output			
$PEC_{oral,fish\ predator,marine}$	concentration in fish-eating predator for marine toppredators	$[kg_c.kg_{wwt}^{-1}]$	O

III.5.1.3 Bioconcentration factor for earthworms

For organic chemicals, the main route of uptake into earthworms will be via the interstitial water. Bioconcentration can be described as a hydrophobic partitioning between the pore water and the phases inside the organism and is modelled according to the equation as described by Jager (1998). The model was supported by data with neutral organic chemicals in soil within the range log Kow 3-8 and in water-only experiments from log Kow 1-6. An application range of log Kow 1-8 is advised and it is reasonable to assume that extrapolation to lower Kow values is possible.

Table III-203 *Default settings for earthworm specific parameters.*

Parameter	**Symbol**	**Unit**	**Value**
Fraction of water inside the worm (volume fraction)	$Fwater_{worm}$	[-]	0.84
Fraction of lipids inside the worm (volume fraction)	$Flipid_{worm}$	[-]	0.012
Density of earthworms	RHO_{worm}	$[kg_{wwt}.m^{-3}]$	1000
Fraction of gut loading in worm	$Fgut_{worm}$	$[kg_{dwt}.kg_{wwt}^{-1}]$	0.1

$$BCF_{worm} = \frac{Fwater_{worm} + Flipid_{worm} \cdot Kow}{RHO_{worm}} \qquad \textbf{(715)}$$

Input

$Fwater_{worm}$	fraction of water inside the worm (volume fraction)	[-]	D
$Flipid_{worm}$	fraction of lipids inside the worm (volume fraction)	[-]	D
Kow	octanol-water partition coefficient	$[m^3.m^{-3}]$	S
RHO_{worm}	density of earthworms	$[kg_{wwt}.m^{-3}]$	D
Output			
BCF_{worm}	bioconcentration factor for earthworms	$[m^3.kg_{wwt}^{-1}]$	O

III.5.1.4 Exposure concentration for worm-eating predators

The concentration in earthworms for secondary poisoning is estimated from the BCF, the gut loading of earthworms and the average of regional and local concentrations in agricultural soil and porewater. The gut loading of earthworms depends heavily on soil conditions and available food. Reported values range from 2-20 % (kg_{dwt} gut/kg_{wwt} voided worm), 10% can therefore be taken as a reasonable value.

$$PEC_{oral,worm} = \frac{0.5 \cdot (PEClocal_{agric,porew} + PECreg_{agric,porew}) \cdot BCF_{worm} + 0.5 \cdot (PEClocal_{agric} + PECreg_{agric}) \cdot Fgut_{worm} \cdot CONV_{soil}}{1 + Fgut_{worm} \cdot CONV_{soil}} \quad \textbf{(716)}$$

Input

$PEClocal_{agric,porew}$	local PEC in pore water of agricultural soil	$[kg_c.m^{-3}]$	O
$PECreg_{agric,porew}$	regional PEC in pore water of agricultural soil	$[kg_c.m^{-3}]$	O
BCF_{worm}	bioconcentration factor for earthworms	$[m^3.kg_{wwt}^{-1}]$	O
$PEClocal_{agric}$	local PEC in agricultural soil (averaged over 180 days)	$[kg_c.kg_{wwt}^{-1}]$	O
$PECreg_{agric}$	regional PEC in agricultural soil	$[kg_c.kg_{wwt}^{-1}]$	O
$Fgut_{worm}$	fraction of gut loading in worm	$[kg_{dwt}.kg_{wwt}^{-1}]$	D
$CONV_{soil}$	conversion factor for soil concentrations: wwt to dwt	$[kg_{wwt}.kg_{dwt}^{-1}]$	O^C

Output

$PEC_{oral,worm}$	concentration in earthworms for secondary poisoning	$[kg_c.kg_{wwt}^{-1}]$	O

III.5.2 Indirect exposure of humans via the environment

Human indirect exposure is assessed by estimating the concentrations and intake of drinking water and food products (root crops, leaf crops, meat, milk and fish). Exposure is estimated on both the local and regional scale. Bioconcentration and biotransfer behaviour is estimated from physico-chemical properties using (Q)SAR approaches. It should be noted that reliable and relevant measured data are always preferable, considering the large uncertainties in the (Q)SARs.

Input: chemical properties			
Kow	octanol-water partition coefficient	[-]	
HENRY	Henry's law constant	[$Pa.m^3.mol^{-1}$]	
$K_{air-water}$	air-water partition coefficient	[$m^3.m^{-3}$]	c
$Fass_{aer}$	fraction of chemical associated with aerosol particles	[-]	
$DT50bio_{water}$	half-life for biodegradation in bulk surface water	[d]	
BCF_{fish}	bioconcentration factor for fish on wet-weight basis	[$m^3.kg_{wwt}^{-1}$]	
Input: local concentrations			
$CONV_{soil}$	conversion factor soil from dry weight to wet weight	[$kg_{wwt}.kg_{dwt}^{-1}$]	c
$PEClocal_{water,ann}$	annual average local PEC in surface water (dissolved)	[$kg_c.m^{-3}$]	
$PEClocal_{air,ann}$	annual average local PEC in air (total)	[$kg_c.m^{-3}$]	
$PEClocal_{grassland}$	local PEC in grassland (total), averaged over 180 days	[$kg_c.kg_{wwt}^{-1}$]	
$PEClocal_{agric,porew}$	local PEC in pore water of agricultural soil	[$kg_c.m^{-3}$]	
$PEClocal_{grassland,porew}$	local PEC in pore water of grassland	[$kg_c.m^{-3}$]	
$PEClocal_{grw}$	local PEC in groundwater under agricultural soil	[$kg_c.m^{-3}$]	
Input: regional concentrations			
$PECreg_{water}$	regional PEC in surface water (dissolved)	[$kg_c.m^{-3}$]	
$PECreg_{air}$	regional PEC in air (total)	[$kg_c.m^{-3}$]	
$PECreg_{agric}$	regional PEC in agricultural soil (total)	[$kg_c.kg_{wwt}^{-1}$]	
$PECreg_{agric,porew}$	regional PEC in pore water of agricultural soils	[$kg_c.m^{-3}$]	

In the regional model, no distinction is made between grassland and other agricultural soils. $PECreg_{agric}$ is also used for the regional grassland concentration. $PECreg_{agric,porew}$ is used for the concentration in groundwater. The indirect exposure calculations are identical for the local and regional scales. Therefore, the indirect exposure equations are described using the following generalised symbols:

Input

C_{water}	concentration in surface water	$[kg_{c}.m^{-3}]$	
C_{air}	concentration in air	$[kg_{c}.m^{-3}]$	
$C_{grassland}$	concentration in grassland soil	$[kg_{c}.kg^{-1}]$	
$C_{agric,porew}$	concentration in pore water of agricultural soil	$[kg_{c}.m^{-3}]$	
$C_{grassland,porew}$	concentration in pore water of grassland soil	$[kg_{c}.m^{-3}]$	
C_{grw}	concentration in groundwater	$[kg_{c}.m^{-3}]$	

Intermediate results 1

$K_{leaf-air}$	partition coeff. between leaves and air	$[m^{3}.m^{-3}]$	
$K_{plant-water}$	partition coeff. between plant tissue and water	$[m^{3}.m^{-3}]$	
TSCF	transpiration stream concentration factor	[-]	
BAF_{meat}	bioaccumulation factor for meat	$[d.kg_{food}^{-1}]$	
BAF_{milk}	bioaccumulation factor for milk	$[d.kg_{food}^{-1}]$	
F_{pur}	purification factor for surface water	[-]	

Intermediate results 2

C_{fish}	concentration in wet fish	$[kg_{c}.kg_{wwt}^{-1}]$	
$Croot_{plant}$	concentration in root tissue of plant	$[kg_{c}.kg_{wwt}^{-1}]$	
C_{leaf}	concentration in leaves of plant	$[kg_{c}.kg_{wwt}^{-1}]$	
C_{grass}	concentration in grass (wet weight)	$[kg_{c}.kg_{wwt}^{-1}]$	
$Fleaf_{porew}$	fraction of total uptake by crops from pore water	[-]	c
$Fleaf_{air}$	fraction of total uptake by crops from air	[-]	c
$Fgrass_{porew}$	fraction of total uptake by grass from pore water	[-]	c
$Fgrass_{air}$	fraction of total uptake by grass from air	[-]	c
C_{drw}	concentration in drinking water	$[kg_{c}.m^{-3}]$	

Intermediate results 3

C_{meat}	concentration in meat (wet weight)	$[kg_{c}.kg_{wwt}^{-1}]$	
C_{milk}	concentration in milk (wet weight)	$[kg_{c}.kg_{wwt}^{-1}]$	
$Fcattle_{i}$	fraction of total intake by cattle through medium *i* $i \in \{grass,drw,air,soil\}$	[-]	c

Intermediate results 4

$DOSE_{i}$	daily dose through intake of *i*	$[kg_{c}.kg_{bw}^{-1}.d^{-1}]$	
$Fdose_{i}$	fraction of total dose through intake of medium *i* $i \in \{drw,fish,leaf,root,meat,milk,air\}$	[-]	c

Output

$DOSE_{tot}$	total daily intake for humans	$[kg_{c}.kg_{bw}^{-1}.d^{-1}]$	

The following table gives the 'temporary' symbols defined in the indirect exposure calculations, and the corresponding specific local and regional symbols.

Temporary symbol	**Local concentration**	**Regional concentration**
C_{water}	$PEClocal_{water,ann}$	$PECreg_{water}$
C_{air}	$PEClocal_{air,ann}$	$PECreg_{air}$
$C_{grassland}$	$PEClocal_{grassland}$	$PECreg_{agric}$
$C_{agric,porew}$	$PEClocal_{agric,porew}$	$PECreg_{agric,porew}$
$C_{grassland,porew}$	$PEClocal_{grassland,porew}$	$PECreg_{agric,porew}$
C_{grw}	$PEClocal_{grw}$	$PECreg_{agric,porew}$

Temporary symbol	Local concentration	Regional concentration
C_{fish}	$Clocal_{fish}$	$Creg_{fish}$
C_{leaf}	$Clocal_{leaf}$	$Creg_{leaf}$
C_{grass}	$Clocal_{grass}$	$Creg_{grass}$
$Fleaf_{porew}$	$Flocal\text{-}leaf_{porew}$	$Freg\text{-}leaf_{porew}$
$Fleaf_{air}$	$Flocal\text{-}leaf_{air}$	$Freg\text{-}leaf_{air}$
$Fgrass_{porew}$	$Flocal\text{-}grass_{porew}$	$Freg\text{-}grass_{porew}$
$Fgrass_{air}$	$Flocal\text{-}grass_{air}$	$Freg\text{-}grass_{air}$
C_{root}	$Clocal_{root}$	$Creg_{root}$
C_{meat}	$Clocal_{meat}$	$Creg_{meat}$
C_{milk}	$Clocal_{milk}$	$Creg_{milk}$
C_{drw}	$Clocal_{drw}$	$Creg_{drw}$
$DOSE_i$	$DOSElocal_i$	$DOSEreg_i$
$Fdose_i$	$Fdose\text{-}local_i$	$Fdose\text{-}reg_i$
$DOSE_{tot}$	$DOSElocal_{tot}$	$DOSEreg_{tot}$

III.5.2.1 Concentration in fish

The BCF for fish is estimated in Section III.5.1.1 on secondary poisoning. The concentration in fish for human indirect exposure is given by:

$$C_{fish} = BCF_{fish} \cdot C_{water} \qquad (717)$$

Input

BCF_{fish}	bioconcentration factor for fish on wet-weight basis	$[m^3.kg_{wwt}^{-1}]$	O
C_{water}	concentration in surface water	$[kg_c.m^{-3}]$	O

Output

C_{fish}	concentration in wet fish	$[kg_c.kg_{wwt}^{-1}]$	O

III.5.2.2 Concentration in crops

The modelling approach proposed by Trapp and Matthies (1995) is used to estimate levels in plants due to uptake from pore water and air (gas phase). This approach integrates uptake from pore water and air into a consistent, one-compartment model. The sink term in the model is formed by diffusive transfer from leaf to air, elimination in the plant tissue, and dilution by growth; the source term is formed by the uptake and translocation from soil and gaseous uptake from air. Aerosol deposition is not considered in the model. Several plant-specific defaults are required, which are summarised in Table III-204.

Table III-204 *Default settings for plant-specific parameters.*

Plant properties, taken from Riederer (1990), values for *Brassica oleracea* (rounded)			
Parameter	**Symbol**	**Unit**	**Value**
Volume fraction of water in plant tissue	$Fwater_{plant}$	$[m^3.m^{-3}]$	0.65
Volume fraction of lipids in plant tissue	$Flipid_{plant}$	$[m^3.m^{-3}]$	0.01
Volume fraction of air in plant tissue	$Fair_{plant}$	$[m^3.m^{-3}]$	0.30
Bulk density of plant tissue	RHO_{plant}	$[kg_{wwt}.m^{-3}]$	700
Plant properties, taken from Trapp and Matthies (1995), values referenced to 1 m^2			
Parameter	**Symbol**	**Unit**	**Value**
Leaf surface area	$AREA_{plant}$	$[m^2]$	5
Conductance (0.001 $m.s^{-1}$)	g_{plant}	$[m.d^{-1}]$	86.4
Shoot volume	V_{leaf}	$[m^3]$	0.002
Transpiration stream (1 $l.d^{-1}$)	Qtransp	$[m^3.d^{-1}]$	1.10^{-3}
Correction exponent for differences between plant lipids and octanol	B	[-]	0.95
Growth-rate constant for dilution by growth	$Kgrowth_{plant}$	$[d^{-1}]$	0.035
Pseudo-first-order rate constant for metabolism	$Kmetab_{plant}$	$[d^{-1}]$	0
Pseudo-first-order rate constant for photodegradation	$Kphoto_{plant}$	$[d^{-1}]$	0

The general partitioning between water and plant tissue is assumed to be based on hydrophobic sorption to plant lipids. *Kow* is corrected slightly for the differences between plant lipids and octanol.

$$K_{plant-water} = Fwater_{plant} + Flipid_{plant} \cdot Kow^{b} \qquad \textbf{(718)}$$

Input			
$Fwater_{plant}$	volume fraction of water in plant tissue	$[m^3.m^{-3}]$	D
$Flipid_{plant}$	volume fraction of lipids in plant tissue	$[m^3.m^{-3}]$	D
Kow	octanol-water partition coefficient	$[m^3.m^{-3}]$	S
b	correction for differences between plant lipids and octanol	[-]	D
Output			
$K_{plant-water}$	partition coeff. between plant tissue and water	$[m^3.m^{-3}]$	O

The concentration in root tissue is governed mainly by physical sorption, and is given by:

$$C_{root} = \frac{K_{plant\text{-}water} \cdot C_{agric,porew}}{RHO_{plant}} \qquad \textbf{(719)}$$

Input			
$K_{plant-water}$	partition coeff. between plant tissue and water	$[m^3.m^{-3}]$	O
$C_{agric,porew}$	concentration in pore water of agricultural soil	$[kg_c.m^{-3}]$	O
RHOplant	bulk density of plant tissue (wet weight)	$[kg_{wwt}.m^{-3}]$	D
Output			
C_{root}	concentration in root tissue of plant	$[kg_c.kg_{wwt}^{-1}]$	O

The transpiration-stream concentration factor (*TSCF*) is the ratio between the concentration in the transpiration stream and the concentration in pore water. *TSCF* is given by (Briggs *et al.*, 1982). This estimation of *TSCF* was derived for a small group of pesticides in one plant species (Barley). Domain of physico-chemical properties: log *Kow* -0.5 to 4.5 (outside this range the minimum or maximum *Kow* is used).

$$TSCF = 0.784 \cdot \exp\left[\frac{-(\log Kow - 1.78)^2}{2.44} \right] \qquad \textbf{(720)}$$

Input			
Kow	octanol-water partition coefficient	[-]	S
Output			
TSCF	transpiration-stream concentration factor	[-]	O

Gaseous exchange between leaves and air can be described by a leaf-air partition coefficient. $K_{leaf\text{-}air}$ is given by:

$$K_{leaf\text{-}air} = Fair_{plant} + \frac{K_{plant\text{-}water}}{K_{air\text{-}water}} \qquad (721)$$

Input

$K_{plant\text{-}water}$	partition coefficient between plant tissue and water	$[m^3.m^{-3}]$	O
$K_{air\text{-}water}$	air-water partition coefficient	$[m^3.m^{-3}]$	O^c
$Fair_{plant}$	volume fraction of air in plant tissue	$[m^3.m^{-3}]$	D
Output			
$K_{leaf\text{-}air}$	partition coeff. between leaves and air	$[m^3.m^{-3}]$	O

Elimination of the substance may take place in the leaf tissue by metabolism or photolysis. If rate constants are known for these processes, they may be added:

$$kelim_{plant} = kmetab_{plant} + kphoto_{plant} \qquad (722)$$

Input

$kmetab_{plant}$	rate constant for metabolism in plants	$[d^{-1}]$	D
$kphoto_{plant}$	rate constant for photolysis in plants	$[d^{-1}]$	D
Output			
$kelim_{plant}$	rate constant for total elimination in plants	$[d^{-1}]$	O^c

The actual one-compartment model for calculating the concentration in the leaf can be described with a simple differential equation. The sink term is formed by diffusive transfer from leaf to air, elimination in the plant tissue and dilution by growth:

$$ALPHA = \frac{AREA_{plant} \cdot g_{plant}}{K_{leaf\text{-}air} \cdot V_{leaf}} + kelim_{plant} + kgrowth_{plant} \qquad (723)$$

Input

$AREA_{plant}$	leaf surface area	$[m^2]$	D
g_{plant}	conductance	$[m.d^{-1}]$	D
$K_{leaf\text{-}air}$	partition coeff. between leaves and air	[-]	O
V_{leaf}	shoot volume	$[m^3]$	D
$kelim_{plant}$	rate constant for elimination in plants	$[d^{-1}]$	O^c
$kgrowth_{plant}$	rate constant for dilution by growth	$[d^{-1}]$	D
Output			
ALPHA	sink term of differential equation	$[d^{-1}]$	O^c

The source term is formed by the uptake and translocation from soil and gaseous uptake from air. Since we have two pore-water concentrations, for agricultural soil and grassland, two separate source terms must be estimated. At the moment, the same default plant characteristics are used for grass as for crops.

$$BETA_{agric} = C_{agric,porew} \cdot TSCF \cdot \frac{Qtransp}{V_{leaf}} + (1 - Fass_{aer}) \cdot C_{air} \cdot g_{plant} \cdot \frac{AREA_{plant}}{V_{leaf}} \quad (724)$$

$$BETA_{grass} = C_{grassland,porew} \cdot TSCF \cdot \frac{Qtransp}{V_{leaf}} + (1 - Fass_{aer}) \cdot C_{air} \cdot g_{plant} \cdot \frac{AREA_{plant}}{V_{leaf}} \quad (725)$$

Input			
Qtransp	transpiration stream	$[m^3.d^{-1}]$	D
$C_{agric,porew}$	concentration in pore water of agricultural soil	$[kg_c.m^{-3}]$	O
$C_{grassland,porew}$	concentration in pore water of grassland	$[kg_c.m^{-3}]$	O
C_{air}	concentration in air	$[kg_c.m^{-3}]$	O
g_{plant}	leaf conductance	$[m.d^{-1}]$	D
TSCF	transpiration-stream concentration factor	[-]	O
V_{leaf}	shoot volume	$[m^3]$	D
$Fass_{aer}$	fraction of substance adsorbed to aerosol	[-]	O
Output			
$BETA_{agric}$	source term of differential equation for crops	$[kg_c.m^{-3}.d^{-1}]$	O^c
$BETA_{grass}$	source term of differential equation for grass	$[kg_c.m^{-3}.d^{-1}]$	O^c

The steady-state concentration is calculated as the source term divided by the sink term. The default growth-dilution rate constant ensures that a steady state will always be reached within the relevant period of time (assuming constant exposure levels).

$$C_{leaf} = \frac{BETA_{agric}}{ALPHA} \cdot \frac{1}{RHO_{plant}} \quad (726)$$

$$C_{grass} = \frac{BETA_{grass}}{ALPHA} \cdot \frac{1}{RHO_{plant}} \quad (727)$$

Input			
ALPHA	sink term of differential equation	$[d^{-1}]$	O^c
$BETA_{agric}$	source term of differential equation, agricultural soil	$[kg_c.m^{-3}.d^{-1}]$	O^c
$BETA_{grass}$	source term of differential equation, grassland	$[kg_c.m^{-3}.d^{-1}]$	O^c
RHO_{plant}	bulk density of plant tissue (wet weight)	$[kg_{wwt}.m^{-3}]$	D
Output			
C_{leaf}	concentration in leaves of plant	$[kg_c.kg_{wwt}^{-1}]$	O
C_{grass}	concentration in grass	$[kg_c.kg_{wwt}^{-1}]$	O

As additional information, the contribution of uptake from pore water and air to the total uptake is calculated.

$$Fleaf_{porew} = \frac{C_{agric,porew} \cdot TSCF \cdot \dfrac{Qtransp}{V_{leaf}}}{BETA_{agric}} \tag{728}$$

$$Fleaf_{air} = \frac{(1 - Fass_{aer}) \cdot C_{air} \cdot g_{plant} \cdot \dfrac{AREA_{plant}}{V_{leaf}}}{BETA_{agric}} \tag{729}$$

$$Fgrass_{porew} = \frac{C_{grassland,porew} \cdot TSCF \cdot \dfrac{Qtransp}{V_{leaf}}}{BETA_{grass}} \tag{730}$$

$$Fgrass_{air} = \frac{(1 - Fass_{aer}) \cdot C_{air} \cdot g_{plant} \cdot \dfrac{AREA_{plant}}{V_{leaf}}}{BETA_{grass}} \tag{731}$$

Input			
Qtransp	transpiration stream	$[m^3.d^{-1}]$	D
$C_{agric,porew}$	concentration in pore water of agricultural soil	$[kg_c.m^{-3}]$	O
$C_{grassland,porew}$	concentration in pore water of grassland	$[kg_c.m^{-3}]$	O
C_{air}	concentration in air	$[kg_c.m^{-3}]$	O
TSCF	transpiration-stream concentration factor	[-]	O
V_{leaf}	shoot volume	$[m^3]$	D
$Fass_{aer}$	fraction of substance adsorbed to aerosol	[-]	O
$BETA_{agric}$	source term of differential equation for crops	$[kg_c.m^{-3}.d^{-1}]$	O^c
$BETA_{grass}$	source term of differential equation for grass	$[kg_c.m^{-3}.d^{-1}]$	O^c
Output			
$Fleaf_{porew}$	fraction of total uptake by crops from pore water	[-]	O^c
$Fleaf_{air}$	fraction of total uptake by crops from air	[-]	O^c
$Fgrass_{porew}$	fraction of total uptake by grass from pore water	[-]	O^c
$Fgrass_{air}$	fraction of total uptake by grass from air	[-]	O^c

III.5.2.3 Concentration in meat and milk products

Travis and Arms (1988) performed a log-linear regression analysis on experimentally derived bioaccumulation factors and the octanol-water partition coefficient. It should be noted that the uncertainty in these estimates is considerable. The concentrations in meat and milk are calculated by applying the bioaccumulation factors and summing the contributions from air, soil, grass and drinking water. The BAF for meat is derived from data on 36 organic compounds, with a log *Kow* range of 1.5 - 6.5. The BAF for milk was derived from data on 28 organic compounds, with a log *Kow* range of 3 - 6.5. Outside these ranges, the minimum or maximum *Kow* is used.

Table III-205 *Default intake rates for cattle.*

Parameter	**Symbol**	**Unit**	**Value**
Daily intake for cattle of grass (dry weight)	$ICdwt_{grass}$	$[kg_{dwt}.d^{-1}]$	16.9 [a]
Daily intake for cattle of soil (dry weight)	$ICdwt_{soil}$	$[kg_{dwt}.d^{-1}]$	0.41 [a]
Daily inhalation rate for cattle	IC_{air}	$[m^3.d^{-1}]$	122 [a]
Daily intake for cattle of drinking water	IC_{drw}	$[m^3.d^{-1}]$	0.055 [b]
Conversion dry weight to wet weight grass	$CONV_{grass}$	$[kg_{wwt}.kg_{dwt}^{-1}]$	4 [a]

[a] Source: McKone and Ryan (1989).
[b] Source: ECETOC (1990).

$$BAF_{meat} = 10^{-7.6 + \log Kow} \tag{732}$$

$$BAF_{milk} = 10^{-8.1 + \log Kow} \tag{733}$$

Input

Kow	octanol-water partition coefficient	[-]	S

Output

BAF_{meat}	bioaccumulation factor for meat	$[d.kg_{meat}^{-1}]$	O
BAF_{milk}	bioaccumulation factor for milk	$[d.kg_{milk}^{-1}]$	O

The default intake rates for soil and grass are expressed as dry weights. These are converted to wet weights as follows:

$$IC_{grass} = ICdwt_{grass} \cdot CONV_{grass} \tag{734}$$

$$IC_{soil} = ICdwt_{soil} \cdot CONV_{soil} \tag{735}$$

Input

$ICdwt_{grass}$	daily intake for cattle of grass (dry weight)	$[kg_{wwt}.d^{-1}]$	D
$CONV_{grass}$	conversion factor grass from dry weight to wet weight	$[kg_{wwt}.kg_{dwt}^{-1}]$	D
$ICdwt_{soil}$	daily intake of soil (dry weight)	$[kg_{wwt}.d^{-1}]$	D
$CONV_{soil}$	conversion factor soil from dry weight to wet weight	$[kg_{wwt}.kg_{dwt}^{-1}]$	O[c]

Output

IC_{grass}	daily intake of grass (wet weight)	$[kg_{wwt}.d^{-1}]$	O[c]
IC_{soil}	daily intake of soil (wet weight)	$[kg_{wwt}.d^{-1}]$	O[c]

The concentrations in meat and milk are calculated as:

$$C_{milk} = BAF_{milk} \cdot \sum C_i \cdot IC_i \quad i \in \{grass, grassland \setminus soil, air, drw\} \tag{736}$$

$$C_{meat} = BAF_{meat} \cdot \sum C_i \cdot IC_i \quad i \in \{grass, grassland \setminus soil, air, drw\} \tag{737}$$

The contribution of each exposure medium to the intake of cattle can be calculated as:

$$Fcattle_i = \frac{C_i \cdot IC_i}{\Sigma C_i \cdot IC_i} \quad i \in \{grass, grassland \setminus soil, air, drw\} \tag{738}$$

Input			
C_{grass}	concentration in grass (wet weight)	$[kg_c.kg_{wwt}^{-1}]$	O
IC_{grass}	daily intake of grass (wet weight)	$[kg_{wwt}.d^{-1}]$	O^c
$C_{grassland}$	total concentration in grassland soil (wet weight)	$[kg_c.kg_{wwt}^{-1}]$	O
IC_{soil}	daily intake of soil (wet weight)	$[kg_{wwt}.d^{-1}]$	O^c
C_{air}	total concentration in air	$[kg_c.m_{air}^{-3}]$	O
IC_{air}	daily inhalation rate of cattle	$[m_{air}^{3}.d^{-1}]$	D
C_{drw}	concentration in drinking water	$[kg_c.m_{drw}^{-3}]$	O
IC_{drw}	daily intake of drinking water	$[m_{drw}^{3}.d^{-1}]$	D
Output			
C_{meat}	concentration in meat (wet weight)	$[kg_c.kg_{wwt}^{-1}]$	O
C_{milk}	concentration in milk (wet weight)	$[kg_c.kg_{wwt}^{-1}]$	O
$Fcattle_i$	fraction of total intake by cattle through *i* $i \in \{grass, soil, air, drw\}$	[-]	O^c

III.5.2.4 Concentration in drinking water

Drinking water is produced from surface water or groundwater. Complete removal of suspended particles from surface water and groundwater is assumed. The effects of the treatment processes used for purification of groundwater, which are generally not intended for the removal of organic pollutants, can be neglected. Surface-water treatment is estimated according to Hrubec and Toet (1992). For the purification of river water for drinking water, a combination of extended storage of river water and extensive treatment is used. The storage is realised in open reservoirs and by means of artificial water recharge in the dunes. Dependent on the type of storage, two different water-treatment systems for surface water can be distinguished:

- System 1:
  - Storage in open reservoirs (volatilisation);
  - Coagulation, flocculation and rapid sand filtration;
  - Active carbon filtration.
- System 2:
  - Coagulation, flocculation and rapid sand filtration;
  - Dune water recharge;
  - Slow sand filtration.

The removal by ozonation of system 1 is not considered, because of the high uncertainty in the removal efficiency of this process. For dune recharge the purification step with powdered activated carbon was not considered (Hrubec and Toet, 1992). Removal of the dissolved fraction of a xenobiotic from the surface water is modelled by means of purification factors. Purification factors for both treatment systems can be taken from Table III-206. Sorption (sedimentation), volatilisation and biodegradation predominantly influence the behaviour of organic compounds during treatment. Hence, the purification factors are dependent on Kow, Henry coefficient and DT50 water. The factors from each relevant column of the table should be multiplied to give a resulting purification factor for each separate system ($Fsys1_{pur}$ and $Fsys2_{pur}$). The maximum value of both systems (worst-case approach) is taken for the purification factor (F_{pur}).

Table III-206 *Purification factors, based on Henry's law constant and biodegradation rate.*

Treatment process	**log *Kow***			**Henry's law constant** *HENRY* ($Pa \cdot m^3 \cdot mol^{-1}$)		**Aerobic biodegradation rate** $DT50bio_{water}$ (days)	
	≤4	4-5	>5	≤100	>100	>10	≤10
System 1	1	1/4	1/16	1	1/2	1	1
System 2	1	1/2	1/4	1	1/2	1	1/4

Source: Hrubec and Toet (1992).

$$F_{pur} = max\,(Fsys1_{pur}\,, Fsys2_{pur}\,) \qquad \textbf{(739)}$$

Input

Kow	octanol-water partition coefficient	[-]	S
HENRY	Henry's law constant	$[Pa.m^3.mol^{-1}]$	O
$DT50bio_{water}$	half-life for biodegradation in bulk surface water	[d]	O
$Fsys1_{pur}$	purification factor for system 1	[-]	O^c
$Fsys2_{pur}$	purification factor for system 2	[-]	O^c

Output

F_{pur}	purification factor for surface water	[-]	O

For the choice between surface water and groundwater, a worst-case approach is followed.

$$C_{drw} = \max\,(C_{water} \cdot F_{pur}\,, C_{grw}) \qquad \textbf{(740)}$$

Input

F_{pur}	purification factor for surface water	[-]	O
C_{water}	dissolved concentration in surface water	$[kg_c.m^{-3}]$	O
C_{grw}	groundwater concentration	$[kg_c.m^{-3}]$	O

Output

C_{drw}	concentration in drinking water	$[kg_c.m^{-3}]$	O

III.5.2.5 Total daily intake for humans

The indirect exposure of humans to chemicals originates from several sources. The exposure assessment includes six pathways: drinking water, fish, crops, meat, milk and air. The daily dose for humans is calculated by means of the concentrations in these media and the daily intake values. This approach implies an exposure scenario whereby each of these intake media is retrieved exclusively from within the contaminated system.

$$DOSE_j = \frac{C_j \cdot IH_j}{BW} \qquad j \in \{drw, fish, leaf, root, meat, milk\} \tag{741}$$

$$DOSE_{air} = \frac{F_{resp} \cdot C_{air} \cdot IH_{air}}{BW} \cdot \frac{BIO_{inh,2}}{BIO_{oral,2}} \tag{742}$$

The total dose can now be calculated as the sum of the dose for each medium:

$$DOSE_{tot} = \sum_i DOSE_i \qquad i \in \{air, drw, fish, leaf, root, meat, milk\} \tag{743}$$

The contribution of each intake medium to the total dose is calculated as:

$$Fdose_i = \frac{DOSE_i}{\sum_i DOSE_i} \tag{744}$$

Input			
C_{drw}	concentration in drinking water	$[kg_c.m^{-3}]$	O
C_{fish}	concentration in fish	$[kg_c.kg_{wwt}^{-1}]$	O
C_{leaf}	concentration in leaves of crops	$[kg_c.kg_{wwt}^{-1}]$	O
C_{root}	concentration in roots of crops	$[kg_c.kg_{wwt}^{-1}]$	O
C_{meat}	concentration in meat	$[kg_c.kg_{wwt}^{-1}]$	O
C_{milk}	concentration in milk	$[kg_c.kg_{wwt}^{-1}]$	O
C_{air}	concentration in air	$[kg_c.m_{air}^{-3}]$	O
F_{resp}	respirable fraction of inhaled substance	[-]	D
IH_i	daily intake of medium *i*	$[kg.d^{-1}$ or $m^3.d^{-1}]$	D
$BIO_{oral,2}$	bioavailability for oral intake	[-]	D
$BIO_{inh,2}$	bioavailability for inhalation	[-]	D
BW	body weight of (adult) human considered	[kg]	D
Output			
$DOSE_i$	daily dose via intake of *i*	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O^c
$DOSE_{tot}$	total daily intake for humans	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$Fdose_i$	fraction of total dose via intake of medium *i*	[-]	O^c

In Table III-207, the default consumption rates for each food product are given (taken from ECETOC, 1994). These values represent the highest country-average intake across all EU Member States for each food product.

Table III-207 *Standard defaults for indirect exposure of humans.*

Parameter	**Symbol**	**Value**	**Unit**	**Source**
Daily intake of drinking water	IH_{drw}	0.002	$[m^3.d^{-1}]$	(b)
Daily intake of fish	IH_{fish}	0.115	$[kg_{wwt}.d^{-1}]$	(a)
Daily intake of leaf crops (incl. fruit and cereals)	IH_{leaf}	1.20	$[kg_{wwt}.d^{-1}]$	(a)
Daily intake of root crops	IH_{root}	0.384	$[kg_{wwt}.d^{-1}]$	(a)
Daily intake of meat	IH_{meat}	0.301	$[kg_{wwt}.d^{-1}]$	(a)
Daily intake of dairy products	IH_{milk}	0.561	$[kg_{wwt}.d^{-1}]$	(a)
Daily inhalation rate	IH_{air}	20	$[m^3.d^{-1}]$	(b)
Respirable fraction of the inhaled substance	F_{resp}	1	[-]	
Bioavailability for inhalation	BIO_{inh}	0.75	[-]	(c)
Bioavailability for oral uptake	BIO_{oral}	1.0	[-]	(c)
Body weight of adult	BW	70	[kg]	

[a] Source: Euromonitor (1992) as reported by ECETOC (1994).
[b] Source: US-EPA (1989).
[c] Source: Vermeire *et al.* (1993b).

III.5.3 Consumer exposure

Five different consumer exposure scenarios are implemented in EUSES:

- Inhalation: a substance that is released as a gas, vapour or airborne particulate into a room (e.g. a component of an aerosol insecticide, a carrier/solvent in a cosmetic formulation, a powder detergent). Release may be the result of direct release as a gas, vapour or particulate, or by evaporation from liquid or solid matrices. In the latter case, the equation represent a worst-case situation by assuming that the substance is directly available as a gas or vapour.
- Dermal a: a substance contained in a medium. This dermal scenario also applies to i) a non-volatile substance in a medium used without further dilution (set dilution *D*=1), and ii) a non-volatile substance in a volatile medium.
- Dermal b: a non-volatile substance migrating from an article (e.g. dyed clothing, residual fabric conditioner, dyestuff/newsprint from paper).
- Oral a: a substance in a product unintentionally swallowed during normal use (e.g. toothpaste).
- Oral b: a substance migrating from an article into food or drink (e.g. plastic film, plastic-coated cups/plates).

Input: inhalation

Q_{prod}	amount of product released	[kg]
Fc_{prod}	weight fraction of substance in product	[-]
V_{room}	room size	$[m^3]$
$T_{contact}$	duration of contact per event	[d]
n	mean number of events per day	$[d^{-1}]$
TIMESCALE	time scale of exposure: acute or (sub-)chronic	[acute/chronic]

Output: inhalation

I_{inh}	inhalatory intake of substance	$[kg_c.kg_{bw}{}^{-1}.d^{-1}]$
C_{inh}	concentration in air of room	$[kg_c.m^{-3}]$

Input: dermal a

n	mean number of events per day	$[d^{-1}]$
C_{prod}	concentration of substance in product before dilution	$[kg_c.m^{-3}]$
D	dilution factor	[-]
RHO_{prod}	density of product before dilution	$[kg_c.m-^3]$
Fc_{prod}	weight fraction of substance in product before dilution	[-]
Q_{prod}	amount of product used	[kg]
V_{prod}	volume of product used before dilution	$[m^3]$
V_{appl}	volume of diluted product actually contacting skin	$[m^3]$
TH_{der}	thickness of product layer on skin	[m]
$AREA_{der}$	area of contact between product and skin	$[m^2]$
TIMESCALE	time scale of exposure: acute or (sub-)chronic	[acute/chronic]

Output: dermal a

C_{der}	dermal concentration of substance on skin	$[kg_c.m^{-3}]$
A_{der}	amount of substance on skin per event	$[kg_c]$
$U_{der,pot}$	amount of substance that can potentially be taken up	$[kg_c.kg_{bw}{}^{-1}.d^{-1}]$

Input: dermal b

C_{prod}	concentration of substance in product before dilution	$[kg_c.m^{-3}]$
RHO_{prod}	density of product before dilution	$[kg.m^{-3}]$
Fc_{prod}	weight fraction of substance in product before dilution	[-]
Q_{prod}	amount of product used	[kg]
V_{prod}	volume of product used before dilution	$[m^3]$
Fc_{migr}	fraction of substance migrating per unit time	$[kg_c.kg^{-1}.d^{-1}]$

$T_{contact}$	duration of contact per event	[d]
TH_{der}	thickness of product	[m]
W_{der}	weight of substance on skin per event	$[kg_{c}.m^{-2}]$
$AREA_{der}$	area of contact between product and skin	$[m^{2}]$
n	mean number of events per day	$[d^{-1}]$
TIMESCALE	time scale of exposure: acute or (sub-)chronic	[acute/chronic]

Output: dermal b

A_{der}	total amount of compound to which skin is pot. exposed	$[kg_{c}]$
$A_{migr,der}$	amount of substance to which skin is expected to be exposed due to migration	$[kg_{c}]$
$U_{der,pot}$	potential uptake	$[kg_{c}.kg_{bw}^{-1}.d^{-1}]$

Input: oral a

C_{prod}	concentration of substance in product before dilution	$[kg_{c}.m^{-3}]$
D	dilution factor	[-]
RHO_{prod}	density of product before dilution	$[kg.m^{-3}]$
Q_{prod}	amount of product before dilution	[kg]
Fc_{prod}	weight fraction of substance in product before dilution	[-]
V_{prod}	volume of product before dilution	$[m^{3}]$
V_{appl}	volume of diluted product in contact with mouth per event	$[m^{3}]$
F_{oral}	fraction of V_{appl} that is ingested	[-]
n	mean number of events per day	$[d^{-1}]$
TIMESCALE	time scale of exposure: acute or (sub-)chronic	[acute/chronic]

Output: oral a

C_{oral}	concentration in ingested product	$[kg_{c}.m^{-3}]$
I_{oral}	intake	$[kg_{c}.kg_{bw}^{-1}.d^{-1}]$

Input: oral b

$AREA_{art}$	surface area of article in contact with food	$[m^{2}]$
TH_{art}	thickness of article in contact with food	[m]
C_{art}	concentration of substance in article	$[kg_{c}.m^{-3}]$
Fc_{migr}	fraction migrating per time	$[kg_{c}.d^{-1}]$
V_{prod}	volume of food	$[m^{3}]$
$T_{contact}$	duration of contact between article and food	[d]
n	mean number of events per day	$[d^{-1}]$
TIMESCALE	time scale of exposure: acute or (sub-)chronic	[acute/chronic]

Output: oral b

C_{oral}	concentration in ingested product	$[kg_{c}.m^{-3}]$
I_{oral}	intake	$[kg_{c}.kg_{bw}^{-1}.d^{-1}]$

Output: chronic exposure

$C_{inh,ann}$	annual average inhalation exposure concentration	$[kg_{c}.m^{-3}]$
$C_{der,ann}$	annual average dermal exposure concentration	$[kg_{c}.m^{-3}]$
$C_{oral,ann}$	annual average oral exposure concentration	$[kg_{c}.m^{-3}]$

Output: total exposure

U_{tot}	total uptake via different routes	$[kg_{c}.kg_{bw}^{-1}.d^{-1}]$

Table III-208 *Defaults for consumer exposure calculations.*

Parameter	**Symbol**	**Unit**	**Value**
Respirable fraction of the inhaled substance	F_{resp}	[-]	1 [a]
thickness of product	TH_{der}	[m]	1.10^{-4}
Bioavailability for oral intake	BIO_{oral}	[-]	1 [a]
Bioavailability for inhalation	BIO_{inh}	[-]	0.75 [a]
Bioavailability for dermal uptake	BIO_{der}	[-]	1
Ventilation rate of person	IH_{air}	$[m^3.d^{-1}]$	20 [a]
Human body weight	BW	[kg]	70 [a]

[a] Already defined in section on human indirect exposure.

III.5.3.1 Inhalatory Consumer Exposure

A substance that is released as a gas, vapour or airborne particulate into a room (e.g. a component of an aerosol insecticide, a carrier/solvent in a cosmetic formulation, a powder detergent). For a description of the ConsExpo inhalatory models see Van Veen (2001).

Release may be the result of direct release as gas, vapour or particulate, or by evaporation from liquid or solid matrices. In the last case, the equation represent a worst-case situation by assuming that the substance is directly available as a gas or vapour. The equation applies to both volatile substances and airborne particulates. The concentration in air after using an amount Q_{prod} of the product becomes:

$$C_{inh} = \frac{Q_{prod} \cdot Fc_{prod}}{V_{room}} \tag{745}$$

The air concentration C_{inh} results in an inhalatory intake of:

$$I_{inh} = \frac{F_{resp} \cdot C_{inh} \cdot IH_{air} \cdot T_{contact}}{BW} \cdot n \tag{746}$$

Input

Q_{prod}	amount of product released	[kg]	S
Fc_{prod}	weight fraction of substance in product	$[kg_c.kg_{prod}]$	S
V_{room}	room size	$[m^3]$	S
F_{resp}	respirable fraction of inhaled substance	[-]	D
IH_{air}	ventilation rate of person	$[m^3.d^{-1}]$	D
$T_{contact}$	duration of contact per event	[d]	S
BW	body weight	[kg]	D
n	mean number of events per day	$[d^{-1}]$	S
Output			
I_{inh}	inhalatory intake of substance	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
C_{inh}	concentration in air of room	$[kg_c.m^{-3}]$	O

III.5.3.2 Dermal Consumer Exposure

Table III-209 *Mean surface area by body part for the adult male (US-EPA, 1989).*

Body part	**Mean surface area (m^2)**
Head (face)	0.1180
Trunk	0.5690
Upper extremities	0.3190
Arms	0.2280
upper arms	0.1430
Forearms	0.1140
hands (fronts and backs)	0.0840
Lower extremities	0.6360
Legs	0.5060
Thighs	0.1980
lower legs	0.2070
Feet	0.1120
Total	1.9400

A substance contained in a medium.

The concentration in the product as used can be calculated using the following equation. Depending on how the parameters are provided, three analogous calculations are used:

$$C_{der} = \frac{C_{prod}}{D} = \frac{RHO_{prod} \cdot Fc_{prod}}{D} = \frac{Q_{prod} \cdot Fc_{prod}}{V_{prod} \cdot D} \qquad \textbf{(747)}$$

The total amount to which the skin is exposed is then given by (two options, depending on format of available data):

$$A_{der} = C_{der} \cdot V_{appl} = C_{der} \cdot TH_{der} \cdot AREA_{der} \qquad \textbf{(748)}$$

The potential uptake per kilogram body weight per day is derived as:

$$U_{der,pot} = \frac{A_{der} \cdot n}{BW} \qquad \textbf{(749)}$$

The above dermal equations apply also to i) a non-volatile substance in a medium used without further dilution (set dilution *D*=1), and ii) a non-volatile substance in a volatile medium. In the latter case, the concentration C_{der} is valid at the very beginning of exposure only. However, this concentration can still be used to calculate A_{der}, because the substance is non-volatile. The above dermal equations can also be used in the case of a volatile substance, but in that case they represent a worst-case situation. If the duration of contact is specified, a chronic exposure can be calculated by EUSES (equation 221). For a description of the ConsExpo inhalatory models see Van Veen (2001).

Input			
C_{prod}	concentration of substance in product before dilution	$[kg_c.m^{-3}]$	S
D	dilution factor	[-]	S
RHO_{prod}	density of product before dilution	$[kg.m^{-3}]$	S
Q_{prod}	amount of product used	[kg]	S
Fc_{prod}	weight fraction of substance in product before dilution	[-]	S
V_{prod}	volume of product used before dilution	$[m^3]$	S
V_{appl}	volume of diluted product actually contacting the skin	$[m^3]$	S
TH_{der}	thickness of product layer on skin	[m]	D
$AREA_{der}$	area of contact between product and skin	$[m^2]$	P/S
BW	body weight	[kg]	D
n	mean number of events per day	$[d^{-1}]$	S
Output			
C_{der}	dermal concentration of substance on skin	$[kg_c.m^{-3}]$	O
A_{der}	amount of substance on skin per event	$[kg_c]$	O
$U_{der,pot}$	amount of substance that can potentially be taken up	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O

A non-volatile substance migrating from an article (e.g. dyed clothing, residual fabric conditioner, dyestuff/newsprint from paper).

The exposure calculation will involve estimating the amount of substance which will migrate from the area of the article in contact with skin during the time of contact. The concentration in the product as used can be calculated according to Equation (209) in case the density of the product and the fraction of substance in the product are known. Dyestuff levels in fabrics and paper are usually given as weight of product per unit area (e.g. mg/m^2). The total amount is then calculated by multiplying by $AREA_{der}$. The amount to which the skin is exposed is given by

$$A_{der} = W_{der} \cdot AREA_{der} = C_{der} \cdot TH_{der} \cdot AREA_{der} \qquad \textbf{(750)}$$

where $C_{der} \cdot TH_{der}$ is equal to weight per unit of area:

$$W_{der} = C_{der} \cdot TH_{der} \qquad \textbf{(751)}$$

Extractability in simulated body fluids for several classes of dyestuffs and different fabric types has been evaluated by ETAD (1983). For migrating substances, only part of the total amount A_{der} is able to reach the skin. The amount to be used is:

$$A_{migr,der} = A_{der} \cdot Fc_{migr} \cdot T_{contact} \qquad \textbf{(752)}$$

where $Fc_{migr} \cdot T_{contact}$ must be much smaller than 1. The potential uptake per kilogram body weight per day is then derived as:

$$U_{der,pot} = \frac{A_{migr,der} \cdot n}{BW} \qquad \textbf{(753)}$$

It should be noted that EUSES does not check whether the estimated daily uptake exceeds the theoretical maximum. This maximum can be derived from the amount of product used (kg), the concentration of the substance ($kg_c.kg^{-1}$) in the product, the use frequency (d^{-1}) and the bodyweight (kg_{bw}).
EUSES also asks to specify the duraction of contact per event to be able to calculate a chronic dermal exposure.

Input			
Fc_{migr}	fraction of substance migrating per unit time	$[kg_c.kg^{-1}.d^{-1}]$	S
$T_{contact}$	duration of contact per event	[d]	S
TH_{der}	thickness of product	[m]	D
W_{der}	weight of substance on skin per event	$[kg_c.m^{-2}]$	S
$AREA_{der}$	area of contact between product and skin	$[m^2]$	P/S
C_{der}	concentration of substance	$[kg_c.m^{-3}]$	O
BW	body weight	[kg]	D
n	mean number of events per day	$[d^{-1}]$	S
Output			
A_{der}	total amount of comp. to which skin is pot. exposed	$[kg_c]$	O
$A_{migr,der}$	amount of substance to which skin is expected to be exposed due to migration	$[kg_c]$	O
$U_{der,pot}$	potential uptake	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O

III.5.3.3 Oral consumer exposure

A substance in a product unintentionally swallowed during normal use (e.g. toothpaste).
These equations may also be used to estimate exposures arising from ingestion of the non-respirable fraction of inhaled airborne particulates. The concentration in the product as swallowed is calculated from

$$C_{oral} = \frac{C_{prod}}{D} = \frac{RHO_{prod} \cdot Fc_{prod}}{D} = \frac{Q_{prod} \cdot Fc_{prod}}{V_{prod} \cdot D} \qquad \textbf{(754)}$$

and the intake is then given by

$$I_{oral} = \frac{F_{oral} \cdot V_{appl} \cdot C_{oral} \cdot n}{BW} \qquad \textbf{(755)}$$

If an undiluted product is swallowed, *D* = 1.
For a description of the ConsExpo inhalatory models see Van Veen (2001).

Input			
C_{prod}	concentration of substance in product before dilution	$[kg_c.m^{-3}]$	S
D	dilution factor	[-]	S
RHO_{prod}	density of product before dilution	$[kg.m^{-3}]$	S
Q_{prod}	amount of product before dilution	$[kg_c]$	S
Fc_{prod}	weight fraction of substance in product before dilution	[-]	S
V_{prod}	volume of product before dilution	$[m^3]$	S
V_{appl}	volume of diluted product per event in contact with mouth	$[m^3]$	S
F_{oral}	fraction of V_{appl} that is ingested	[-]	S
BW	body weight	[kg]	D
n	mean number of events per day	$[d^{-1}]$	S
Output			
C_{oral}	concentration in ingested product	$[kg_c.m^{-3}]$	O
I_{oral}	intake	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O

A substance migrating from an article into food or drink (e.g. plastic film, plastic-coated cups/plates).

The following equation can be used to obtain a conservative estimate of substance uptake from a defined volume of food. The value of Fc_{migr} will be influenced by the type of food (e.g. fatty/dry/moist), the period of exposure and the temperature at which migration occurs. The consumer exposure level will be influenced by the proportion of the contaminated food eaten. The concentration in the food as a result of migration from an article is given by:

$$C_{oral} = \frac{AREA_{art} \cdot TH_{art} \cdot C_{art} \cdot Fc_{migr} \cdot T_{contact}}{V_{prod}} \tag{756}$$

Oral intake is given by:

$$I_{oral} = \frac{V_{appl} \cdot C_{oral} \cdot n}{BW} \tag{757}$$

Input			
$AREA_{art}$	surface area of article in contact with food	$[m^2]$	S
TH_{art}	thickness of article in contact with food	[m]	S
C_{art}	concentration of substance in article	$[kg_c.m^{-3}]$	S
Fc_{migr}	fraction migrating per time	$[kg_c.d^{-1}]$	S
V_{prod}	volume of food	$[m^3]$	S
V_{appl}	volume of diluted product actually ingested	$[m^3]$	S
$T_{contact}$	contact duration between article and food	[d]	S
BW	body weight	[kg]	D
n	mean number of events per day	$[d^{-1}]$	S
Output			
C_{oral}	concentration in ingested product	$[kg_c.m^{-3}]$	O
I_{oral}	intake	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O

III.5.3.4 Acute versus chronic consumer exposure

Consumer exposure may be acute or chronic. Because consumer products are used lifelong, the lifetime average exposure is well approximated by using the annual average exposure, averaging out seasonal usage differences. With regard to acute exposures, the equations used for consumer exposure model exposures as resulting from a constant concentration, thereby setting mean and maximum event concentrations equal. Therefore, acute exposure is characterized by the inhalatory, dermal, and oral concentrations, C_{inh}, C_{der}, and C_{oral} respectively, which are given in the model descriptions. For chronic exposures, the intake and potential uptake rates I_{inh}, $U_{der,pot}$ and I_{oral} represent annual average measures of exposure. Where chronic exposure is measured with reference to concentration, the annual average exposure concentrations are to be used:

$$C_{route,ann} = \frac{\int_0^{365} C_{route}(t)\,dt}{365} \qquad route \in \{inh, der, oral\} \qquad (758)$$

where C_{route} represents the exposure concentration via the inhalatory, dermal or oral route. Both the acute and the chronic characterisation of exposure are given. The former is compared to the LD50, the latter to the chronic NOAEL. Because the equations model exposure with reference to constant concentration, the equation can be written as:

$$C_{route,ann} = C_{route} \cdot n \cdot T_{contact} \qquad route \in \{inh, der, oral\} \qquad (759)$$

Input			
C_{route}	exposure concentration through route *route*	$[kg_c.m^{-3}]$	O
$T_{contact}$	event duration	[d]	S
n	mean number of events per day	$[d^{-1}]$	S
Output			
$C_{inh,ann}$	annual average inhalation exposure concentration	$[kg_c.m^{-3}]$	O
$C_{der,ann}$	annual average dermal exposure concentration	$[kg_c.m^{-3}]$	O
$C_{oral,ann}$	annual average oral exposure concentration	$[kg_c.m^{-3}]$	O

Both the acute and the chronic characterisations are given per route. The acute concentrations are compared to the appropriate acute toxicity value, the chronic intakes or concentrations to the appropriate N(L)OAEL.

III.5.3.5 Total consumer exposure

If a consumer is exposed to a substance in a particular consumer product via different routes, the contribution of each route to the total uptake can be summed. The summation is done for each time scale separately (acute and -sub-chronic).

Differences in bioavailability for the various routes are accounted for by multiplying the intakes (or potential uptakes) with absolute absorption factors.

$$U_{tot} = I_{inh} \cdot BIO_{inh,2} + U_{der,pot} \cdot BIO_{der,2} + I_{oral} \cdot BIO_{oral,2} \qquad \textbf{(760)}$$

Input			
I_{inh}	inhalatory intake of substance	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$U_{der,pot}$	potential uptake	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
I_{oral}	intake	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$BIO_{oral,2}$	bioavailability for oral intake (end route)	[-]	D
$BIO_{inh,2}$	bioavailability for inhalation (end route)	[-]	D
$BIO_{der,2}$	bioavailability for dermal uptake (end route)	[-]	D
Output			
U_{tot}	total uptake for one product via different routes	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O

III.5.3.6 ConsExpo

ConsExpo 3.0 (Van Veen, 2001) can be started (or circumvented) from EUSES. When started the selected output of Consexpo is exported to EUSES and used in the further calculation

General input data

With the ConsExpo implements several exposure models for the *inhalatory*, *dermal* and *oral* routes of exposure resp. For all these scenarios the contact of the exposed person with the substance and the physico-chemical properties of the substance have to be defined:

Input: contact	
use frequency	$[year^{-1}]$
use duration	[min]
total duration	[min]
Input: chemical	
molecular weight	$[g.mol^{-1}]$
octanol/water partition coefficient	[number]
vapour pressure	[Pa]
water solubility	$[g.liter^{-1}]$

ConsExpo: inhalatory models

ConsExpo implements the EUSES inhalatory model as the “constant concentration”-scenario. In addition ConsExpo implements five more advanced inhalatory scenarios.

- source-ventilation : a substance is released into the (ventilated) room air with a constant release rate.
- evaporation from pure substance: a substance is released from a open can filled with the (liquid) substance in it’s pure form by evaporation.
- evaporation from mixture: a substance is released by evaporation from a open can filled with a liquid mixture of which the substance is an ingredient.
- painting: a viscous product such as paint is being applied to a surface with a certain application area. The substance, which is part of the paint, diffuses to the surface of the applied product and evaporates.
- spray: currently being revised.

Input: source and ventilation	
generation (/release) rate of the substance	$[kg_c.s^{-1}]$
break down rate of the substance	$[s^{-1}]$

room volume	[m^{3}]
ventilation rate	[h^{-1}]
ambient air concentration	[kg$_{c}$.m^{-3}]

Input: evaporation from pure substance model

release area	[m^{2}]
temperature	[^{o}C]
room volume	[m^{3}]
ventilation rate	[m^{3}.h^{-1}]

Input: evaporation from mixture model

release area	[m^{2}]
temperature	[^{o}C]
room volume	[m^{3}]
ventilation rate	[h^{-1}]
molecular weight matrix product	[kg.mol^{-1}]
weight fraction of the substance in the product	[fraction]

Input: painting model

release area	[m^{2}]
product amount	[g]
weight fraction of the substance in the product	[fraction]
density product	[kg.m^{-3}]
layer exchange rate	[min^{-1}]
fraction upper layer	[fraction]
room volume	[m^{3}]
ventilation rate	[h^{-1}]
temperature	[^{o}C]
molecular weight matrix product	[kg.mol^{-1}]

Input: spray model
Currently being revised

ConsExpo offers three uptake models to calculate the <u>internal dose</u> for the inhalatory route:

- Fraction model: a (user-)specified fraction of the exposure enters the body
- Diffusion model:
- Flow model

Input: fraction model

inhalation rate	[m3.min-1]
absorbed fraction	[fraction] (should be 1 to calculate potential dose)
respirable fraction	[fraction]

Input: diffusion model

air/blood partition coefficient	[ratio]
blood flow	[cm^{3}.min^{-1}]
volume lung blood	[cm^{3}]
lung wall permeability	[cm.min^{-1}]
lung volume	[liter]
dead space	[fraction]
inhalation rate	[liter.min^{-1}]
respirable fraction	[fraction]

Input: flow model

air/blood partition coefficient	[fraction]
blood flow	[cm^{3}.s^{-1}]
inhalation rate	[liter.min^{-1}]
respirable fraction	[fraction]

ConsExpo: dermal models

In addition to the EUSES dermal a and dermal b models (termed “fixed volume” and “contact rate” model resp.) ConsExpo implements three more detailed dermal scenarios.

- Migration to skin
- Product diffusion
- Transfer coefficient

Input: migration to skin model

fraction of chemical that is leachable	[kg/kg]
product amount	[kg]
fraction of the product that is in direct contact with the skin	[fraction]

Input: product diffusion model

concentration compound	[g.cm^{-3}]
diffusion coefficient of the substance in product	[m^{2}.min^{-1}]
evaporation rate of the substance from the product	[cm.min^{-1}]
thickness product	[cm]

Input: transfer coefficient model

transfer coefficient (area rubbed per unit time)	[cm^{2}.min^{-1}]
dislodgeable amount	[g. cm^{-2}]
weight fraction of the substance	[fraction]
half life chemical	[min]
contaminated surface	[m^{2}]

ConsExpo offers three uptake models to calculate the internal dose for the dermal route:

- Fraction model
- Diffusion model
- SKINPERM model

Input: fraction model

absorped fraction	[fraction] (should be 1 to calculate potential dose)

ConsExpo: oral models

In addition to the EUSES oral a and oral b models (termed “single ingestion” and “article-food migration” model resp.) ConsExpo implements three specific oral scenarios:

- Hand-mouth conact scenario
- Product leaching scenario
- Non-respirable fraction scenario

Input: hand-mouth contact model

concentration of compound in the product on the hands	[g.cm^{-3}]
intake rate of the product	[cm^{3}.min^{-1}]

Input: product leaching model

concentration compound	[g.cm^{-3}]
product volume	[cm^{3}]
leach rate	[g.cm^{-2}.min^{-1}]
area in contact with the mouth	[cm^{2}]

Input: non-respirable fraction model

non-respirable fraction	[fraction]
inhalation rate	[liter.min^{-1}]

In addition to this fraction, a concentration of the substance in air has to be calculated using one of the inhalatory scenarios.

ConsExpo offers two uptake models to calculate the internal dose for the oral route:
- Fraction model
- Diffusion model

Input: fraction model

absorped fraction	[fraction] (should be 1 to calculate potential dose)

ConsExpo output

Existing EUSES output parameter	ConsExpo output	Unit Consexpo	Unit EUSES
Per route			
C_{inh} I_{inh} (if fraction is set to 1 in CONSEXPO)	• Inhalatory exposure as the mean event air concentration of the substance • Inhalatory uptake as the total amount of substance taken up yearly by inhalation (in 'uptake-model' fraction = 1)	$[mg.m^{-3}]$ $[mg.kg_{bw}^{-1}.d^{-1}]$	$[kg_c.m^{-3}]$ $[kg_c.kg_{bw}^{-1}.d^{-1}]$
C_{der} $U_{der,pot}$ (if fraction is set to 1 in CONSEXPO)	• Dermal exposure as the concentration of substance in contact withe skin • Dermal uptake as total amount of substance taken up yearly through the skin (in 'uptake-model' fraction = 1)	$[mg.cm^{-3}]$ $[mg. kg_{bw}^{-1}.d^{-1}]$	$[kg_c.m^{-3}]$ $[kg_c.kg_{bw}^{-1}.d^{-1}]$
C_{oral} I_{oral} (if fraction is set to 1 in CONSEXPO)	• Oral exposure as the concentration of substance that is swallowed • Oral exposure as the total amount of substance taken up yearly (in 'uptake-model' fraction = 1)	$[mg.cm^{-3}]$ $[mg. kg_{bw}^{-1}.d^{-1}]$	$[kg_c.m^{-3}]$ $[kg_c.kg_{bw}^{-1}.d^{-1}]$

III.5.4 Workplace exposure

(Sub)chronic exposure of workers is estimated by means of the model EASE, implemented in EUSES. In addition acute exposure values can be entered by the user. Different scenarios can be assessed for the inhalatory and dermal route and for each scenario a total exposure is calculated. The user needs to provide answers on the questions presented by this model (see decision trees in Appendix IV). Based on the answers, exposure ranges are estimated for inhalatory exposure to vapours, fibers and dust and for dermal exposure. EASE also produces a log file showing a summary of the choices made.

Input		
-	specific questions on exposure (see decision trees in Appendix IV)	
$C_{inh,worker,acute}$	acute inhalation exposure of workers	[kg.m^{-3}]
$W_{der,worker,acute}$	acute dermal weight of substance on skin of workers	[kg.m^{-1}.d^{-1}]
$U_{der,pot,worker,acute}$	acute potential dermal uptake for workers	[kg.kg$_{bw}^{-1}$.d^{-1}]
Intermediate results		
$W_{der,worker}$	dermal weight of substance on skin of workers	[kg.m^{-2}.d^{-1}]
Output		
$C_{inh,worker,vapour}$	vapour concentration in air for workers	[kg$_{c}$.m^{-3}]
$C_{inh,worker,fibre}$	fibre concentration in air for workers	[fibers.m^{-3}]
$C_{inh,worker,dust}$	dust concentration in air for workers	[kg.m^{-3}]
$U_{der,pot,worker}$	potential dermal uptake for workers	[kg.kg$_{bw}^{-1}$.d^{-1}]
-	log file of EASE	

III.5.4.1 Inhalatory worker exposure

Input			
-	specific questions on exposure (see decision trees in Appendix IV)		S
$C_{inh,worker,acute}$	acute inhalation exposure of workers	[kg.m^{-3}]	S
Output			
$C1_{inh,worker,vapour}$	vapour concentration in air for workers (in ppm)	[ppm]	O
$C_{inh,worker,fibre}$	fibre concentration in air for workers	[fibers.m^{-3}]	O
$C_{inh,worker,dust}$	dust concentration in air for workers	[kg.m^{-3}]	O
-	log file of EASE		

Table III-210 *Default for workplace exposure.*

Parameter	**Symbol**	**Unit**	**Value**
Average temperature at the workplace	TEMPwork	[K]	293
Thickness of product layer on skin	$TH_{der,worker}$	[m]	1.10^{-4}
body weight	BW	[kg]	70[a]
respirable fraction of inhaled substance	F_{resp}	[-]	1[a]
ventilation rate of worker	$IH_{air,worker}$	[m^{3}.d^{-1}]	10[b]

[a] Already defined in section on human indirect exposure.
[b] Also used in the section on human effect assessment.

The output of EASE for inhalation exposure of workers to vapour is a range with the unit parts per million (ppm). This formula corrects for the average temperature at the workplace during working hours and applies at a standard pressure of 101.3 kPa. The default temperature is assumed to be 293 K.

$$C_{inh,worker,vapour} = \frac{273}{TEMPwork} \cdot MOLW \cdot 10^{-6} \cdot C1_{inh,worker,vapour} \cdot \frac{1000}{22.4} \qquad (761)$$

Input			
TEMPwork	average temperature on the workplace	[K]	D
MOLW	molecular weight	[$kg_c.mol^{-1}$]	S
$C1_{inh,worker,vapour}$	vapour concentration in air for workers (in ppm)	[ppm]	O
Output			
$C_{inh,worker,vapour}$	vapour concentration in air for workers	[$kg.m^{-3}$]	O

III.5.4.2 Dermal worker exposure

Input			
-	specific questions on exposure (see decision trees in Appendix IV)		S
$W_{der,worker,acute}$	acute dermal weight of substance on skin of workers	[$kg.m^{-1}.d^{-1}$]	S
$U_{der,pot,worker,acute}$	acute potential dermal uptake for workers	[$kg.kg_{bw}^{-1}.d^{-1}$]	S
Output			
$W_{der,worker}$	dermal weight of substance on skin of workers	[$kg.m^{-2}.d^{-1}$]	O
-	log file of EASE		O

Dermal exposure of workers can be estimated as an external weight (kg_c) per unit skin surface area (m^2) per unit of time (d). For the risk characterisation this exposure has to be recalculated to a potential uptake per kg body weight per day:

$$U_{der,worker,pot,acute} = W_{der,worker,acute} \cdot \frac{AREA_{der,worker}}{BW} \qquad (762)$$

$$U_{der,worker,pot} = W_{der,worker} \cdot \frac{AREA_{der,worker}}{BW} \qquad (763)$$

Input			
$AREA_{der,worker}$	area of contact between substance and skin	[m^2]	D
BW	body weight	[kg]	D
$W_{der,worker,acute}$	acute dermal weight of substance on skin of workers	[$kg.m^{-1}.d^{-1}$]	S
$W_{der,worker}$	dermal weight of substance on skin of workers	[$kg.m^{-2}.d^{-1}$]	O
Output			
$U_{der,pot,worker,acute}$	acute potential dermal uptake for workers	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O
$U_{der,pot,worker}$	potential dermal uptake for workers	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O

III.5.4.3 Total worker exposure

If a worker is exposed to a substance via different routes, the contribution of each route to the total uptake can be summed. The summation is done for each time scale separately (acute and – sub-chronic).

Differences in bioavailability for the inhalatory and dermal routes are accounted for by multiplying the intakes (or potential uptakes) with absolute absorption factors.

The vapour exposure concentrations for workers are recalculated to intakes:

$$I_{inh,worker,acute} = \frac{F_{resp} \cdot C_{inh,worker,acute} \cdot IH_{air,worker} \cdot T_{contact,worker}}{BW} \cdot n \qquad \textbf{(764)}$$

$$I_{inh,worker,vapour} = \frac{F_{resp} \cdot C_{inh,worker,vapour} \cdot IH_{air,worker} \cdot T_{contact,worker}}{BW} \cdot n \qquad \textbf{(765)}$$

Input

F_{resp}	respirable fraction of inhaled substance	[-]	D
$IH_{air,worker}$	ventilation rate of worker	[$m^3.d^{-1}$]	D
$T_{contact,worker}$	duration of contact with skin of worker per event	[d]	S
BW	body weight	[kg]	D
n	mean number of events per day	[d^{-1}]	S
$C_{inh,worker,acute}$	acute inhalation exposure of workers	[$kg.m^{-3}$]	S
$C_{inh,worker,vapour}$	vapour concentration in air for workers	[$kg.m^{-3}$]	O

Output

$I_{inh,worker,acute}$	acute inhalatory intake of substance for worker	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O
$I_{inh,worker,\ vapour}$	inhalatory intake of substance for worker	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O

$$U_{tot-v/d,worker} = I_{inh,worker,vapour} \cdot BIO_{inh} + U_{der,pot,worker} \cdot BIO_{der} \qquad \textbf{(766)}$$

$$U_{tot,worker,acute} = I_{inh,worker,acute} \cdot BIO_{inh} + U_{der,pot,worker,acute} \cdot BIO_{der} \qquad \textbf{(767)}$$

Input

$I_{inh,worker,acute}$	acute inhalatory intake of substance for worker	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$I_{inh,worker, vapour}$	inhalatory intake of substance for worker	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
BIO_{inh}	bioavailability for inhalation	[-]	D
BIO_{der}	bioavailability for dermal uptake	[-]	D
$U_{der,pot,worker,acute}$	acute potential dermal uptake for workers	$[kg.kg_{bw}^{-1}.d^{-1}]$	O
$U_{der,pot,worker}$	potential dermal uptake for workers	$[kg.kg_{bw}^{-1}.d^{-1}]$	O

Output

$U_{tot,worker,acute}$	total uptake for one scenario via different routes, for acute effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$U_{tot-v/d,worker}$	total uptake (vapour + dermal) for one scenario via different routes	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O

III.6 EFFECTS ASSESSMENT

III.6.1 Effects assessment for the environment

For the environmental end-points, Predicted No-Effect Concentrations (PNECs) are assessed. For the extrapolation from single-species toxicity tests to the population or ecosystem level, assessment factors are used. A statistical method may be used to support the assessment.

Input: micro-organism effects data			
$EC50_{micro}$	EC50 for STP micro-organisms	$[kg_c.m^{-3}]$	
$EC10_{micro}$	EC10 for STP micro-organisms	$[kg_c.m^{-3}]$	
$NOEC_{micro}$	NOEC for STP micro-organisms	$[kg_c.m^{-3}]$	
Input: aquatic effects data			
$LC50aqua_i$	LC50 for aquatic organisms, trophic level *i*	$[kg_c.m^{-3}]$	
$NOECaqua_i$	NOEC for aquatic organisms, trophic level *i*	$[kg_c.m^{-3}]$	
$LC50aqua_{i,marine}$	LC50 for marine aquatic organisms, trophic level *i*	$[kg_c.m^{-3}]$	
$NOECaqua_{i,marine}$	NOEC for marine aquatic organisms, trophic level *i*	$[kg_c.m^{-3}]$	
Input: terrestrial effects data			
$LC50terr_i$	LC50 for terrestrial organisms, trophic level *i*	$[kg_c.kg_{wwt}^{-1}]$	
$NOECterr_i$	NOEC for terrestrial organisms, trophic level *i*	$[kg_c.kg_{wwt}^{-1}]$	
$K_{soil-water}$	soil-water partition coefficient	$[m^3.m^{-3}]$	c
$K_{sed-water}$	sediment-water partition coefficient	$[m^3.m^{-3}]$	c
RHO_{soil}	bulk density of soil	$[kg_{wwt}.m^{-3}]$	c
Input: bird / mammalian effects data			
$LC50_{bird}$	LC50 in avian dietary study (5 days)	$[kg_c.kg_{food}^{-1}]$	
$NOEC_{bird}$	NOEC for birds	$[kg_c.kg_{food}^{-1}]$	
$NOEC_{mammal,food,chr}$	NOEC for mammals	$[kg_c.kg_{food}^{-1}]$	
$NOAEL_{bird}$	NOAEL for birds	$[kg_c.kg_{bw}.d^{-1}]$	
$NOAEL_{mammal,oral,chr}$	NOAEL for mammals	$[kg_c.kg_{bw}.d^{-1}]$	
T_{bird}	duration of (sub-)chronic test with birds	[d]	
T_{mammal}	duration of (sub-)chronic test with mammals	[d]	
$CONV_{bird}$	conversion factor for NOAEL to NOEC	$[kg_{bw}.d.kg_{food}^{-1}]$	
$CONV_{mammal}$	conversion factor for NOAEL to NOEC	$[kg_{bw}.d.kg_{food}^{-1}]$	

Intermediate results 1			
TOXaqua	toxicological data used for extrapolation of PNEC	[$kg_c.m^{-3}$]	
AFaqua	assessment factor applied in extrapolation of aquatic PNEC	[-]	
$AFaqua_{marine}$	assessment factor applied in extrapolation of marine PNEC	[-]	
TOXmicro	toxicological data used for extrapolation of PNEC	[$kg_c.m^{-3}$]	
AFmicro	assessment factor applied in extrapolation of PNEC	[-]	
TOXoral	toxicological data used for extrapolation of PNEC	[$kg_c.kg_{food}^{-1}$]	
AForal	assessment factor applied in extrapolation of PNEC	[-]	
Intermediate results 2			
TOXterr	toxicological data used for extrapolation of PNEC	[$kg_c.kg_{wwt}^{-1}$]	
AFterr	assessment factor applied in extrapolation of PNEC	[-]	
EPterr	equilibrium partitioning used for PNEC in soil?	[yes/no]	c
EPsed	equilibrium partitioning used for PNEC in sediment?	[yes/no]	c
Output 1			
$PNEC_{water}$	PNEC for aquatic organisms	[$kg_c.m^{-3}$]	c
$PNEC_{water,marine}$	PNEC for marine aquatic organisms	[$kg_c.m^{-3}$]	c
$PNEC_{micro-organisms}$	PNEC for STP micro-organisms	[$kg_c.m^{-3}$]	c
$PNEC_{oral}$	PNEC for secondary poisoning of birds and mammals	[$kg_c.kg_{food}^{-1}$]	c
$PNECstat_{water}$	PNEC for aquatic organisms with statistical method	[$kg_c.m^{-3}$]	c
$PNECstat_{water, marine}$	PNEC for marine aquatic organisms with statistical method	[$kg_c.m^{-3}$]	c
$PNECstat_{soil}$	PNEC for terrestrial organisms with statistical method	[$kg_c.m^{-3}$]	c
Output 2			
$PNEC_{soil}$	PNEC for terrestrial organisms	[$kg_c.kg_{wwt}^{-1}$]	c
$PNEC_{sed}$	PNEC for sediment-dwelling organisms	[$kg_c.kg_{wwt}^{-1}$]	

***Table III-211** Default environmental characteristics soil and sediment in all scales*

Sediment			
Weight fraction of organic carbon soil solids	Foc_{soil}	[$kg_{oc}.kg_{solid}$-1]	0.02
Weight fraction of organic matter soil solids	Fom_{soil}	[$kg_{om}.kg_{solid}$-1]	0.02
Weight fraction of organic carbon in fresh water and marine sediment	Foc_{sed}	[$kg_{oc}.kg_{solid}$-1]	0.05
Weight fraction of organic matter in fresh water and marine sediment	Fom_{sed}	[$kg_{om}.kg_{solid}$-1]	0.05

III.6.1.1 Aquatic compartment (freshwater and marine environment)

Depending on the available toxicity data for aquatic organisms, assessment factors are selected for extrapolating single-species toxicity tests to a PNEC for the water compartment. If intermittent release is identified for a stage of the life cycle, only short-term effects need to be considered for risk characterisation of that stage (only for the aquatic compartment). The following trophic levels are distinguished for the freshwater and marine environment:

- algae (primary producers);
- crustaceans / *Daphnia* (primary consumers);
- fish (secondary consumers);
- other species (e.g. decomposers).

$$LC50\,aqua_{min} = \min\left(LC50\,aqua_i \right) \qquad \textbf{(768)}$$

$$NOECaqua_{min} = \min\left(NOECaqua_i \right) \qquad \textbf{(769)}$$

Table III-212 *Assessment factors for deriving the PNEC*$_{water}$ *for freshwater.*

Available data	**Additional criteria**	**TOXaqua**	**AFaqua**
3 LC50s		$LC50aqua_{min}$	1000
3 LC50s (independent of avail. NOECs)	If intermittent release is identified for a stage of the life cycle	$LC50aqua_{min}$	100
1 NOEC additional (not algae!)	**Same taxonomic group as** $\mathbf{LC50aqua_{min}}$**?** yes no $LC50aqua_{min}/1000 < NOECaqua_{min}/100$ no $LC50aqua_{min}/1000 \geq NOECaqua_{min}/100$	 $NOECaqua_{min}$ $LC50aqua_{min}$ $NOECaqua_{min}$	 100 1000 100
2 NOEC additional	**Same taxonomic group as** $\mathbf{LC50aqua_{min}}$**?** yes no $LC50aqua_{min} < NOECaqua_{min}$ no $LC50aqua_{min} \geq NOECaqua_{min}$	 $NOECaqua_{min}$ $LC50aqua_{min}$ $NOECaqua_{min}$	 50 100 100
3 NOEC algae, *Daphnia* and fish		$NOECaqua_{min}$	10
3 NOEC *not* algae, *Daphnia* and fish	**Same taxonomic group as** $\mathbf{LC50aqua_{min}}$**?** yes No	 $NOECaqua_{min}$ $NOECaqua_{min}$	 10 50
Species Sensitivity Distribution	At least 10 NOECs for species covering at least 8 taxonomic groups	See section III.6.1.6	

The greater diversity of taxa in the marine environment, compared to freshwaters, will produce a broader distribution of species sensitivity. In those cases where only data for freshwater or saltwater algae, crustaceans and fish are available a higher assessment factor should be applied than that for the derivation of PNEC$_{water}$ for freshwaters. This higher assessment factor reflects the greater uncertainty in the extrapolation. Where data is available for additional marine taxonomic groups, for example rotifers, echinoderms or molluscs the uncertainties in the extrapolation are reduced and the magnitude of the assessment factor applied to a data set can be lowered.

Table III-213 *Assessment factors for deriving the PNEC$_{water}$ for the marine environment.*

Available data	**Additional criteria**	**TOXaqua**	**AFaqua marine**
3 LC50s (algae, *Daphnia* or crustaceans, and fish)		LC50aqua$_{min}$	10000 [a]
3 LC50s (algae, *Daphnia* or crustaceans, and fish) and additional 2 LC50s marine (e.g. echinoderms, molluscs)		LC50aqua$_{min}$	1000
1 NOEC additional (not algae!)	**Same taxonomic group as LC50aqua$_{min}$, based on 3 LC50s?**		
	Yes	NOECaqua$_{min}$	1000
	no LC50aqua$_{min}$/10000 < NOECaqua$_{min}$/1000	LC50aqua$_{min}$	10000
	no LC50aqua$_{min}$/10000 ≥ NOECaqua$_{min}$/1000	NOECaqua$_{min}$	1000
2 NOEC additional	**Same taxonomic group as LC50aqua$_{min}$, based on 3 LC50s?**		
	yes and 2 LC50 marine available [b]	NOECaqua$_{min}$	50
	yes and 1 LC50s marine available [b]	NOECaqua$_{min}$	100
	yes and most sensitive species examined [c]	NOECaqua$_{min}$	100
	yes	NOECaqua$_{min}$	500
	no LC50aqua$_{min}$ < NOECaqua$_{min}$	LC50aqua$_{min}$	1000
	no LC50aqua$_{min}$ ≥ NOECaqua$_{min}$	NOECaqua$_{min}$	1000
3 NOEC algae, *Daphnia* or crustaceans, and fish	**Same taxonomic group as LC50aqua$_{min}$, based on 3 LC50s?**		
	Yes	NOECaqua$_{min}$	100 [d]
	no LC50aqua$_{min}$ ≥ NOECaqua$_{min}$	NOECaqua$_{min}$	500
	no LC50aqua$_{min}$ < NOECaqua$_{min}$	LC50aqua$_{min}$	1000
2 NOEC (algae, *Daphnia* or fish) and additional 1 NOEC marine (e.g. echinoderms, molluscs)		NOECaqua$_{min}$	50
3 NOEC (algae, *Daphnia* or fish) and additional 2 NOEC marine (e.g. echinoderms, molluscs)		NOECaqua$_{min}$	10
Species Sensitivity Distribution	At least 10 NOECs for species covering at least 8 taxonomic groups	See section III.6.1.6	

[a] In specific cases this factor can be varied (see TGD). Under no circumstances the AF should be lower than 1000 except if intermittent release is identified for a stage of the life cycle;

[b] A reduced assessment factor of 100 and 50 may be appropriate, when one or two short-term test on marine species *of additional taxonomic groups* (e.g. echinoderms, molluscs) are available, respectively. The short-term marine tests must indicate that they are not from the most sensitive group and it must been determined with a high probability that long-term NOECs generated for these groups would not be lower than already obtained

c It may sometimes be possible to determine with a high probability that, from the two available NOECs, the most sensitive species covering fish, crustacea and algae has been examined. So, a further longer-term NOEC from a third taxonomic group would not be lower than the data already available;

Under specific circumstances this factor may be reduced to a minimum of 10 (see TGD).

$$PNEC_{water} = \frac{TOXaqua}{AFaqua} \tag{770}$$

$$PNEC_{water,marine} = \frac{TOXaqua}{AFaqua_{marine}} \tag{771}$$

Input			
LC50aqua$_{i}$	LC50 for aquatic organisms, trophic level *i*	[kg$_{c}$.m^{-3}]	S
NOECaqua$_{i}$	NOEC for aquatic organisms, trophic level *i*	[kg$_{c}$.m^{-3}]	S
LC50aqua$_{i,marine}$	LC50 for marine aquatic organisms, trophic level *i*	[kg$_{c}$.m^{-3}]	S
NOECaqua$_{i,marine}$	NOEC for marine aquatic organisms, trophic level *i*	[kg$_{c}$.m^{-3}]	S
Output			
LC50aqua$_{min}$	lowest LC50 for aquatic organisms	[kg$_{c}$.m^{-3}]	O
NOECaqua$_{min}$	lowest NOEC for aquatic organisms	[kg$_{c}$.m^{-3}]	O
TOXaqua	toxicological data used for extrapolation of PNEC	[kg$_{c}$.m^{-3}]	O
AFaqua	assessment factor applied in extrapolation of aquatic PNEC	[-]	O
AFaqua$_{marine}$	assessment factor applied in extrapolation of marine PNEC	[-]	O
PNEC$_{water}$	PNEC for aquatic organisms	[kg$_{c}$.m^{-3}]	O^{c}
PNEC$_{water,marine}$	PNEC for marine aquatic organisms	[kg$_{c}$.m^{-3}]	O^{c}

III.6.1.2 Terrestrial compartment

For most chemicals, the number of toxicity data on soil organisms will be limited. At base-set level, there is no requirement for toxicity tests with soil organisms, except for some Product Types in the Biocides Directive. When no toxicity data are available, equilibrium partitioning will be applied. It should be noted that in case of intermittent release, the equilibrium partitioning method must depart from the PNEC based on chronic effects and not the PNEC derived from LC50s.

If only one test result for soil organisms is available, the lowest of the PNECs resulting from the equilibrium partitioning and assessment factor approach is used. Depending on the toxicity data available for terrestrial organisms, assessment factors are selected for extrapolating single-species toxicity tests to a PNEC for the soil compartment. The following trophic levels are distinguished:

- plants (primary producers);
- earthworms (consumers);
- micro-organisms (decomposers);
- others.

Natural soils used in ecotoxicological tests differ in characteristics such as organic matter and clay content, soil pH and soil moisture content. The bioavailability of the test compound, and therefore the toxicity observed, is influenced by these soil properties. This means that results from different test soils cannot be compared directly. If possible data should be normalised using relationships that describes the bioavailability of chemicals in soils. Results are converted to a standard soil, which is defined as a soil with an organic matter content of 3.4% or an organic carbon content of 2.0% (see section III.4.1).

$$Foc_{soil} = Fom_{soil} / 1.7 \tag{772}$$

$$LC50terr_{standard,i} = LC50terr_i \cdot \frac{Foc_{soil}}{Foc_{soil,exp}} \tag{773}$$

$$NOECterr_{standard,i} = NOECterr_i \cdot \frac{Foc_{soil}}{Foc_{soil,exp}} \tag{774}$$

$$LC50\,terr_{min} = \min\left(LC50\,terr_{standard,i} \right) \tag{775}$$

$$NOECterr_{min} = \min\left(NOECterr_{standard,i} \right) \tag{776}$$

$$PNEC_{soil,ep} = \frac{K_{soil\text{-}water}}{RHO_{soil}} \cdot PNEC_{water} \tag{777}$$

***Table III-214** Assessment factors for deriving the $PNEC_{soil}$ for the terrestrial environment.*

Available ecotox. data	**Additional criteria**	**TOXterr**	**AFterr**
none		$PNEC_{soil,ep}$	1
1 LC50	$PNEC_{soil,ep} < LC50terr_{min}/1000$ $PNEC_{soil,ep} \geq LC50terr_{min}/1000$	$PNEC_{soil,ep}$ $LC50terr_{min}$	1 1000
>1 LC50		$LC50terr_{min}$	1000
1 NOEC no LC50s	$PNEC_{soil,ep} < NOECterr_{min}/100$ $PNEC_{soil,ep} \geq NOECterr_{min}/100$	$PNEC_{soil,ep}$ $NOECterr_{min}$	1 100
1 NOEC and >0 LC50s	$LC50terr_{min}/1000 < NOECterr_{min}/100$ $LC50terr_{min}/1000 \geq NOECterr_{min}/100$	$LC50terr_{min}$ $NOECterr_{min}$	1000 100
2 NOEC	**NOEC's of two taxonomic groups?**		
	Yes No	$NOECterr_{min}$ $NOECterr_{min}$	50 100
3 NOEC	**NOEC's of three taxonomic groups?**		
	Yes No	$NOECterr_{min}$ $NOECterr_{min}$	10 50
Species Sensitivity Distribution	At least 10 NOECs for species covering at least 8 taxonomic groups	See section III.6.1.6	

$$PNEC_{soil} = \frac{TOXterr}{AFterr} \qquad (778)$$

If $TOXterr = PNEC_{soil,ep}$ then $EPterr$ = 'yes'

Input

Foc_{soil}	weight fraction of organic carbon in soil	$[kg.kg^{-1}]$	D
Fom_{soil}	weight fraction of organic matter in soil	$[kg.kg^{-1}]$	D/O
$Foc_{soil,exp}$	weight fraction of organic carbon in tested soil	$[kg.kg^{-1}]$	S
$LC50terr_i$	LC50 for terrestrial organisms, trophic level *i*	$[kg_c.kg_{wwt}^{-1}]$	S
$NOECterr_i$	NOEC for terrestrial organisms, trophic level *i*	$[kg_c.kg_{wwt}^{-1}]$	S
$LC50terr_{standard,i}$	Standardised LC50 for terrestrial organisms, trophic level *i*	$[kg_c.kg_{wwt}^{-1}]$	S/O
$NOECterr_{standard,i}$	Standardised NOEC for terrestrial organisms, trophic level *i*	$[kg_c.kg_{wwt}^{-1}]$	S/O
$PNEC_{water}$	PNEC for aquatic organisms	$[kg_c.m^{-3}]$	O^c
$K_{soil-water}$	soil-water partition coefficient	$[m^3.m^{-3}]$	O^c
RHO_{soil}	bulk density of soil	$[kg_{wwt}.m^{-3}]$	O^c
$PNEC_{soil,ep}$	PNEC for terrestrial organisms derived by eq. part.	$[kg_c.kg_{wwt}^{-1}]$	O^c

Output

TOXterr	toxicological data used for extrapolation of PNEC	$[kg_c.kg_{wwt}^{-1}]$	O
AFterr	assessment factor applied in extrapolation of PNEC	[-]	O
EPterr	equilibrium partitioning used for PNEC?	[yes/no]	O^c
$PNEC_{soil}$	PNEC for terrestrial organisms	$[kg_c.kg_{wwt}^{-1}]$	O^c

III.6.1.3 Sediment compartment (freshwater and marine environment)

For most chemicals the number of toxicity data on sediment-dwelling organisms will be limited. For the initial risk assessment, normally no effect data from tests with sediment-dwelling organisms will be available. Therefore, the equilibrium-partitioning approach is implemented in EUSES. It should be noted that in case of intermittent release, the equilibrium partitioning method must depart from the PNEC based on chronic effects and not the PNEC derived from LC50s.

If one or more acute toxicity tests for sediment-dwelling organisms is/are available, the lowest of the PNECs resulting from the equilibrium partitioning and assessment factor approach is used. Depending on the toxicity data available for sediment-dwelling organisms, assessment factors are selected for extrapolating single-species toxicity tests to a PNEC for the sediment compartment.

In contrast with the other PNECs, the PNEC for sediment is an open parameter to allow for expert estimation from available data outside EUSES.

$$LC50sed_{min} = \min\left(LC50sed_i \right) \tag{779}$$

$$NOECsed_{min} \ or \ EC10sed_{min} = \min\left(NOECsed_i \ or \ EC10sed_i \right) \tag{780}$$

$$PNEC_{sed,ep} = \frac{K_{susp-water}}{RHO_{susp}} \cdot PNEC_{water} \tag{781}$$

Table III-215 *Assessment factors for deriving the PNEC$_{sediment}$ for freshwater environment.*

Available ecotox. Data	**Additional criteria**	**TOXterr**	**AFterr**
None		PNEC$_{sed,ep}$	1
≥1 LC50	PNEC$_{sed,ep}$ < LC50sed$_{min}$/10000 PNEC$_{sed,ep}$ ≥ LC50sed$_{min}$/10000	PNEC$_{sed,ep}$ LC50sed$_{min}$	1 1000
1 NOEC/EC10		NOECsed$_{min}$/ EC10sed$_{min}$	100
2 NOEC/EC10	With species representing different living and feeding conditions	NOECsed$_{min}$/ EC10sed$_{min}$	50
3 NOEC/EC10	With species representing different living and feeding conditions	NOECsed$_{min}$/ EC10sed$_{min}$	10

For the marine effect assessment of sediment-dwelling organisms attention should be paid to the fact that very often contaminants are not analysed in whole sediment but in a certain fraction of the sediment, for example in the sediment fraction of particles < 63 μm. The organic carbon content of this fraction is typically 15-30% for marine sediment while for whole marine sediments it is generally less than 2%. It is important, for reasons of comparability of PEC and PNEC values, that the organic carbon content of sediment used for toxicity tests are comparable with those of actual marine sediments. Results for marine and freshwater sediments should be converted to a standard sediment, which is defined as a sediment with an organic matter content of 8.5% or an organic carbon content of 5.0% (see section III.4.1).

$$LC50sed_{standard,i} = LC50sed_i \cdot \frac{Foc_{sed}}{Foc_{sed,exp}} \qquad \textbf{(782)}$$

$$NOECsed_{standard,i} = NOECsed_i \cdot \frac{Foc_{sed}}{Foc_{sed,exp}} \qquad \textbf{(783)}$$

$$PNEC_{sed,marine,ep} = \frac{K_{susp\text{-}water}}{RHO_{susp}} \cdot PNEC_{water,marine} \qquad \textbf{(784)}$$

Table III-216 *Assessment factors for deriving the PNEC$_{sediment}$ for marine environment.*

Available ecotox. Data	**Additional criteria**	**TOXterr**	**AFterr**[a]
None		$PNEC_{sed,marine,ep}$	1
1 LC50 (marine or freshwater organism)	$PNEC_{sed,marine,ep} < LC50sed_{min}/1000$ $PNEC_{sed,marine,ep} \geq LC50sed_{min}/10000$	$PNEC_{sed,marine,ep}$ $LC50sed_{min}$	1 10000
2 LC50 (incl. one marine organism of sensitive taxa)	$PNEC_{sed,marine,ep} < LC50sed_{min}/1000$ $PNEC_{sed,marine,ep} \geq LC50sed_{min}/1000$	$PNEC_{sed,marine,ep}$ $LC50sed_{min}$	1 1000
1 NOEC/EC10		$NOECsed_{min}$/ $EC10sed_{min}$	1000
2 NOEC/EC10	With species representing different living and feeding conditions	$NOECsed_{min}$/ $EC10sed_{min}$	500
1 NOEC/EC10 and additional 1 NOEC/EC10 marine	With species representing different living and feeding conditions	$NOECsed_{min}$/ $EC10sed_{min}$	100
3 NOEC/EC10	With species representing different living and feeding conditions	$NOECsed_{min}$/ $EC10sed_{min}$	50
1 NOEC/EC10 and additional 2 NOEC/EC10 marine	With species representing different living and feeding conditions	$NOECsed_{min}$/ $EC10sed_{min}$	10
3 NOEC/EC10 marine	With species representing different living and feeding conditions	$NOECsed_{min}$/ $EC10sed_{min}$	10

[a] Where there is convincing evidence that the sensitivity of marine organisms is adequately covered by that available from freshwater species, the assessment factors used for freshwater sediment data may be applied. Such evidence may include data from long-term testing of freshwater and marine aquatic organisms, and must include data on specific marine taxa.

$$PNEC_{sed} = \frac{TOXsed}{AFsed} \qquad (785)$$

$$PNEC_{sed,marine} = \frac{TOXsed}{AFsed_{marine}} \qquad (786)$$

If $TOXsed = PNEC_{sed,ep}$ then $EPsed$ = 'yes'

Input			
Foc_{sed}	weight fraction of organic carbon in marine sediment	$[kg.kg^{-1}]$	D
Fom_{sed}	weight fraction of organic matter in marine sediment	$[kg.kg^{-1}]$	D/O
$Foc_{sed,exp}$	weight fraction of organic carbon in tested sediment	$[kg.kg^{-1}]$	S
$LC50sed_i$	LC50 for sediment-dwelling organisms, species *i*	$[kg_c.kg_{wwt}^{-1}]$	S
$NOECsed_i$	NOEC for sediment-dwelling organisms, species *i*	$[kg_c.kg_{wwt}^{-1}]$	S
$EC10sed_i$	EC10 for sediment-dwelling organisms, species *i*	$[kg_c.kg_{wwt}^{-1}]$	S
$LC50sed_{standard,i}$	Standardised LC50 for sediment-dwelling organisms, species *i*	$[kg_c.kg_{wwt}^{-1}]$	S/O
$NOECsed_{standard,i}$	Standardised NOEC for sediment-dwelling organisms, species *i*	$[kg_c.kg_{wwt}^{-1}]$	S/O
$EC10sed_{standard,i}$	Standardised EC10 for sediment-dwelling organisms, species *i*	$[kg_c.kg_{wwt}^{-1}]$	S/O
$PNEC_{water}$	PNEC for aquatic organisms	$[kg_c.m^{-3}]$	O^c
$K_{susp-water}$	suspended matter-water partition coefficient	$[m^3.m^{-3}]$	O^c
RHO_{susp}	bulk density of suspended matter	$[kg_{wwt}.m^{-3}]$	O^c
$PNEC_{sed,ep}$	PNEC for sediment-dwelling organisms derived by eq. part.	$[kg_c.kg_{wwt}^{-1}]$	O^c
Output			
TOXsed	toxicological data used for extrapolation of PNEC	$[kg_c.kg_{wwt}^{-1}]$	O
AFsed	assessment factor applied in extrapolation of PNEC	[-]	O
EPsed	equilibrium partitioning used for PNEC in sediment?	[yes/no]	O^c
$PNEC_{sed}$	PNEC for sediment-dwelling organisms	$[kg_c.kg_{wwt}^{-1}]$	O

III.6.1.4 Micro-organisms

Chemicals may cause adverse effects on microbial activity in STPs and therefore it is necessary to derive a PNECmicro-organisms. Current test systems for measuring the effect of chemicals on microbial activity have different endpoints and different levels of sensitivity. A number of internationally accepted test systems exist. Available data suggest the following order of increasing sensitivities among particular test systems: respiration inhibition test < inhibition control in base-set tests < growth inhibition test with P. putida < inhibition of nitrification. Depending on the test system and toxicity data available for micro-organisms, assessment factors are selected for extrapolating results from toxicity tests to a PNEC for the sewage treatment plant.

Table III-217 *Assessment factors for deriving the PNEC$_{micro-organisms}$ for the STP.*

Test system	**TOXmicro**	**AFmicro**
Activated sludge, respiration inhibition tests		
Respiration inhibition tests EU Annex V C.11, OECD 209	$NOEC_{micro}$ or $EC10_{micro}$	10
	$EC50_{micro}$	100
Inhibition control in base-set tests		
Inhibition control in standard biodegradation test: ready or inherent tests	Tested conc. at which toxicity to inoculum can be ruled out [a]	10
Activated sludge, other tests		
Activated sludge growth inhibition tests, ISO-15522	$NOEC_{micro}$ or $EC10_{micro}$	10
	$EC50_{micro}$	100
Pilot scale activated sludge simulation tests OECD 303 A, ISO-11733	Expert judgement [b]	Case-by-case down to 1
Tests with specific populations of bacteria or protozoa		
Inhibition of nitrification, ISO-9509	$NOEC_{micro}$ or $EC10_{micro}$	1
	$EC50_{micro}$	10
Ciliate growth inhibition tests,	$NOEC_{micro}$ or $EC10_{micro}$	1
	$EC50_{micro}$	10
Growth inhibition tests with *Pseudomonas putida,* NF EN ISO 10712	$NOEC_{micro}$ or $EC10_{micro}$	1
	$EC50_{micro}$	10

[a] The tested concentration at which toxicity to the inoculum can be ruled out with sufficient reliability (cf. corresponding text section above) could be considered as a NOEC for the toxicity to micro-organisms of a STP;

[b] Based on case-by-case expert judgement, the tested concentration not impairing proper functioning of the continuous activated sludge unit could be considered as NOEC for micro-organisms in STPs

If more than one toxicity value is given, the lower of the resulting PNECs is used.

$$PNEC_{micro-organisms} = \frac{TOXmicro}{AFmicro} \qquad (787)$$

Input			
$EC50_{micro}$	EC50 for STP micro-organisms	$[kg_c.m^{-3}]$	S
$EC10_{micro}$	EC10 for STP micro-organisms	$[kg_c.m^{-3}]$	S
$NOEC_{micro}$	NOEC for STP micro-organisms	$[kg_c.m^{-3}]$	S
Output			
TOXmicro	toxicological data used for extrapolation of PNEC	$[kg_c.m^{-3}]$	O
AFmicro	assessment factor applied in extrapolation of PNEC	[-]	O
$PNEC_{micro\text{-}organisms}$	PNEC for STP micro-organisms	$[kg_c.m^{-3}]$	O^c

III.6.1.5 Secondary poisoning

For new substances, the results of mammalian repeated-dose toxicity test(s) are used to assess secondary poisoning effects. For existing substances, toxicity data for birds may also be present. Extrapolation from such test results gives a predicted no-effect concentration in food that should be protective of other mammalian and avian species. Acute lethal doses LD50 (rat, bird) are not acceptable for extrapolation to chronic toxicity, as these tests are not dietary tests. Acute effect concentrations (LC50, 5-day avian dietary studies) for birds are acceptable for extrapolation. The results of these tests may be expressed as a concentration in the food (mg/kg) or a dose (mg/kg body weight/day) causing no effect. For the assessment of secondary poisoning, the results are converted to the concentration in food (kg_c/kg food). NOECs converted from NOAELs have the same priority as direct NOECs. The table below gives some conversion factors for laboratory species.

Bird toxicity tests are not usually given for the test durations specified below (T_{bird}). This test duration is however only used to arrive at a representative assessment factor. The user therefore has to decide whether a longer-term bird toxicity test is comparable to 90 day or chronic mammal test.

Table III-218 *Assessment factors for deriving the $PNEC_{oral}$ for secondary poisoning.*

Available ecotox. Data	**Duration of (sub-)chronic test**	**TOXoral**	**AForal**
$LC50_{bird}$ only	5 days	$LC50_{bird}$	3000
$NOEC_{bird}$	Chronic	$NOEC_{bird}$	30
$NOEC_{mammal,food,chr}$	28 days 90 days chronic	$NOEC_{mammal,food,chr}$	300 90 30

If an NOEC for both birds and mammals is given, the lower of the resulting PNECs is used.

$$PNEC_{oral} = \frac{TOXoral}{AForal} \tag{788}$$

Input			
$LC50_{bird}$	LC50 in avian dietary study (5 days)	$[kg_c.kg_{food}^{-1}]$	S
$NOEC_{bird}$	NOEC for birds	$[kg_c.kg_{food}^{-1}]$	S/O
$NOEC_{mammal,food,chr}$	NOEC for mammals	$[kg_c.kg_{food}^{-1}]$	S/O
T_{bird}	duration of (sub-)chronic test with birds	[d]	P
T_{mammal}	duration of (sub-)chronic test with mammals	[d]	P
Output			
TOXoral	toxicological data used for extrapolation of PNEC	$[kg_c.kg_{food}^{-1}]$	O
AForal	assessment factor applied in extrapolation of PNEC	[-]	O
$PNEC_{oral}$	PNEC for secondary poisoning of birds and mammals	$[kg_c.kg_{food}^{-1}]$	O^c

If toxicity data are given as NOAEL only:

$$NOEC_{bird} = NOAEL_{bird} \cdot CONV_{bird} \tag{789}$$

$$NOEC_{mammal,\, food,chr} = NOAEL_{mammal,oral,chr} \cdot CONV_{mammal} \tag{790}$$

Input			
$NOAEL_{bird}$	NOAEL for birds	$[kg_c.kg_{bw}.d^{-1}]$	S
$NOAEL_{mammal,oral,chr}$	NOAEL for mammals	$[kg_c.kg_{bw}.d^{-1}]$	S/O
$CONV_{bird}$	conversion factor from NOAEL to NOEC	$[kg_{bw}.d.kg_{food}^{-1}]$	S
$CONV_{mammal}$	conversion factor from NOAEL to NOEC	$[kg_{bw}.d.kg_{food}^{-1}]$	P/S
Output			
$NOEC_{bird}$	NOEC for birds	$[kg_c.kg_{food}^{-1}]$	S/O
$NOEC_{mammal,food,chr}$	NOEC for mammals	$[kg_c.kg_{food}^{-1}]$	S/O

The conversion factors as published in the TGD and reproduced in Table III-219, with the addition of the factor for Guinea pig, can be traced back to Lehman (1954) and Romijn et al. (1993) and are based on default assumptions for body weights and daily food consumption. Other, more detailed values for body weights and food consumption can be found in the TGD, Part I, Appendix VI.

Table III-219 *Conversion factors from NOAEL to NOEC for several mammalian species.*

Species	**Conversion factor (BW/DFI)** **$CONV_{mammal}$ [$kg_{bw}.d.kg_{food}^{-1}$]**
*Canis domesticus/*dog	40
*Cavia cobaya/*Guinea pig	25
*Cricetus/*hamster	10
Macaca spp./*monkey*	20
Microtus spp./vole	8.3
*Mus musculus/*mouse	8.3
*Oryctolagus cuniculus/*rabbit	33.3
Rattus norvegicus (> 6 weeks)/rat	20
Rattus norvegicus (≤ 6 weeks)/rat	10
*Gallus domesticus/*chick	8

III.6.1.6 Statistical extrapolation method

The statistical extrapolation method itself is not incorporated in EUSES 2.0.
The Aldenberg and Jaworska (2000) method within the ETX-program (Van Vlaardingen and Traas, 2002) can be used to support the effect assessment performed with assessment factors. The results of this method can be entered as input ($PNEC_{stat}$). For the statistical extrapolation method we refer to the ETX-program, which can be obtained from the RIVM (info@rivm.nl).

The no-effect level (HC_5) calculated according the Aldenberg and Jaworska (2000) method within ETX is the median concentration with the 90% confidence interval that protects 95% of the species in the system for which the experimental NOECs are a representative sample. The method is used for aquatic as well as terrestrial toxicity data. Values of the extrapolation constant k_s depend on the number of NOECs given and the desired confidence level. According to the TGD (2003) at least 10 NOECs from at least 8 different taxonomic groups must be present for this calculation. The TGD lists the taxonomical groups that are required. The TGD also documents data selection and data averaging, if more than one NOEC is available for each species.

In ETX it is checked whether the toxicity data deviate from the assumed normal distribution using the Anderson-Darling test (and the Kolmogorov Smirnov test). If a test statistic is above the 5% critical value, normality is rejected at the 5% critical value, indicating doubts about normality. If a GOF test statistic is below the 5% critical value, normality is accepted at the 5% critical value. If a higher critical value is accepted (e.g. at 2.5% significance level), then the probability that these data derive from a normal distribution is smaller than at 5%, but it is not impossible that the sample derives from a normal distribution. A GOF test does *not* say that a sample cannot derive from a normal distribution, just that it becomes less probable with decreasing significance levels.

Input

$PNECstat_{water}$	PNEC for aquatic organisms with statistical method	$[kg_c.m^{-3}]$	S
$PNECstat_{water, marine}$	PNEC for marine aquatic organisms with statistical method	$[kg_c.m^{-3}]$	S
$PNECstat_{soil}$	PNEC for terrestrial organisms with statistical method	$[kg_c.m^{-3}]$	S

III.6.1.7 PBT assessment

The PBT assessment (persistence, bioconcentration, toxicity) is not included in EUSES. It is referred to the TGD (2003) (Part II, chapter 4.4) for the criteria and the testing strategies.

III.6.2 Effects assessment for humans

III.6.2.1 Route-to-route extrapolation

For acute time scale effects it is not common to perform route-to-route extrapolations. When necessary and applicable, for (sub-)chronic time scale effects (repeated dose toxicity, carcinogenicity and reproductive toxicity (and within this endpoint a.o. fertility, maternal toxicity and developmental toxicity) route-to-route extrapolations may be performed.

Oral-to-dermal route

If oral and dermal absorption rates are known these should be used in the calculations. If these data are not known default values should be taken.

Table III-220 *Defaults for oral-to-dermal extrapolation.*

Parameter	**Symbol** [(a)]	**Unit**	**Value**
Bioavailability for oral uptake	$BIO_{oral,1}$	[-]	1
Bioavailability for dermal uptake	$BIO_{der,2}$	[-]	
MOLW >500 and [log Kow <-1 or >4]			0.10
MOLW ≤500 and [log Kow ≥-1 or ≤4]			1

These are parameters are already defined in the sub-modules on human exposure.

(a) “1” indicates starting route, “2” end route.

$$NOAEL_{mammal,der,i} = NOAEL_{mammal,oral,i} \cdot \frac{BIO_{oral,1}}{BIO_{der,2}} \tag{791}$$

$$LOAEL_{mammal,der,i} = LOAEL_{mammal,oral,i} \cdot \frac{BIO_{oral,1}}{BIO_{der,2}} \tag{792}$$

$$NOAEL_{man,der,i} = NOAEL_{man,oral,i} \cdot \frac{BIO_{oral,1}}{BIO_{der,2}} \tag{793}$$

$$LOAEL_{man,der,i} = LOAEL_{man,oral,i} \cdot \frac{BIO_{oral,1}}{BIO_{der,2}} \tag{794}$$

$$CED_{mammal,der,i} = CED_{mammal,oral,i} \cdot \frac{BIO_{oral,1}}{BIO_{der,2}} \tag{795}$$

$$i \in \{repdose, carc, fert, mattox, devtox\}$$

$$T25_{mammal,der,nt} = T25_{mammal,oral,nt} \cdot \frac{BIO_{oral,1}}{BIO_{der,2}} \tag{796}$$

$$CED_{mammal,der,nt} = CED_{mammal,oral,nt} \cdot \frac{BIO_{oral,1}}{BIO_{der,2}} \tag{797}$$

If absorption rates of humans and experimental animals differ and are known, the toxicity parameter estimated by EUSES should be corrected manually by multiplication with a factor $BIO_{der\text{-}animal}/BIO_{der\text{-}human}$.

Input			
$N(L)OAEL_{mammal,oral,i}$	oral N(L)OAEL for mammals for endpoint *i*	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$N(L)OAEL_{man,oral,i}$	oral N(L)OAEL for man for endpoint *i*	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$T25_{mammal,oral,nt}$	oral T25 for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,oral,i}$	oral CED for mammals for endpoint i $i \in$ {repdose,carc,fert,mattox,devtox}	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,oral,\ nt}$	oral CED for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$BIO_{oral,1}$	bioavailability for oral uptake (starting route)	[-]	S/D
$BIO_{der,2}$	bioavailability for dermal uptake (end route)	[-]	S/D
Output			
$N(L)OAEL_{mammal,der,i}$	dermal N(L)OAEL for mammals for endpoint *i*	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$N(L)OAEL_{man,der,i}$	dermal N(L)OAEL for man for endpoint *i* $i \in$ {repdose,carc,fert,mattox,devtox}	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$T25_{mammal,der,nt}$	dermal T25 for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,der,i}$	dermal CED for mammals for endpoint i $i \in$ {repdose,carc,fert,mattox,devtox}	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,der,\ nt}$	dermal CED for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O

Oral-to-inhalatory route

If oral and inhalation absorption rates are known these should be used in the calculations. If these data are not known default values should be taken. To err on the side of caution, the default value for the starting route (oral) is 50%. The respiratory rate used has to fulfill the requirements of allometric scaling and therefore the inhalatory rate (of humans) is multiplied with the allometric correction factor (AFallom). The TGD proposes the following values: rat 4, mice 7, guinea pig 3, rabbit 2.4, monkey 2, dog 1.4.

$$NOAEL_{mammal,inh,i} = NOAEL_{mammal,oral,i} \cdot \frac{BW}{IH_{air} \cdot AF_{allom}} \cdot \frac{BIO_{oral,1}}{BIO_{inh,2}} \tag{798}$$

$$LOAEL_{mammal,inh,i} = LOAEL_{mammal,oral,i} \cdot \frac{BW}{IH_{air} \cdot AF_{allom}} \cdot \frac{BIO_{oral,1}}{BIO_{inh,2}} \tag{799}$$

$$NOAEL_{man,inh,i} = NOAEL_{man,oral,i} \cdot \frac{BW}{IH_{air} \cdot AF_{allom}} \cdot \frac{BIO_{oral,1}}{BIO_{inh,2}} \tag{800}$$

$$LOAEL_{man,inh,i} = LOAEL_{man,oral,i} \cdot \frac{BW}{IH_{air} \cdot AF_{allom}} \cdot \frac{BIO_{oral,1}}{BIO_{inh,2}} \tag{801}$$

$$CED_{mammal,inh,i} = CED_{mammal,oral,i} \cdot \frac{BW}{IH_{air} \cdot AF_{allom}} \cdot \frac{BIO_{oral,1}}{BIO_{inh,2}} \tag{802}$$

$$i \in \{repdose, carc, fert, mattox, devtox\}$$

$$T25_{mammal,inh,nt} = T25_{mammal,oral,nt} \cdot \frac{BW}{IH_{air} \cdot AF_{allom}} \cdot \frac{BIO_{oral,1}}{BIO_{inh,2}} \tag{803}$$

$$CED_{mammal,inh,nt} = CED_{mammal,oral,nt} \cdot \frac{BW}{IH_{air} \cdot AF_{allom}} \cdot \frac{BIO_{oral,1}}{BIO_{inh,2}} \tag{804}$$

If absorption rates of humans and experimental animals differ and are known, the toxicity parameter estimated by EUSES should be corrected manually by multiplication with a factor $BIO_{inh-animal}/BIO_{inh-human}$.

Table III-221 *Defaults for oral-to-inhalation extrapolation.*

Parameter	**Symbol** (a)	**Unit**	**Value**
Bioavailability for oral uptake	$BIO_{oral,1}$	[-]	0.50
Bioavailability for inhalation	$BIO_{inh,2}$	[-]	1
Body weight of the human considered	BW	$[kg_{bw}]$	70
Daily inhalation rate Consumer / Humans via the environment	IH_{air}	$[m^3.d^{-1}]$	20

These are parameters are already defined in the sub-modules on human exposure.
(a) "1" indicates starting route, "2" end route.

Input

$N(L)OAEL_{mammal,oral,i}$	oral N(L)OAEL for mammals for endpoint *i*	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$N(L)OAEL_{man,oral,i}$	oral N(L)OAEL for man for endpoint *i*	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$T25_{mammal,oral,nt}$	oral T25 for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,oral,i}$	oral CED for mammals for endpoint i $i \in$ {repdose,carc,fert,mattox,devtox}	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,oral, nt}$	oral CED for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$BIO_{oral,1}$	bioavailability for oral uptake (starting route)	[-]	S/D
$BIO_{inh,2}$	bioavailability for inhalation (end route)	[-]	S/D
BW	body weight of the human considered	$[kg_{bw}]$	D
IH_{air}	daily inhalation rate of humans	$[m^3.d^{-1}]$	D
AF_{allom}	allometric scaling factor	[-]	D

Output

$N(L)OAEL_{mammal,inh,i}$	inhalatory N(L)OAEL for mammals for endpoint *i*	$[kg_c.m^{-3}]$	S/O
$N(L)OAEL_{man,inh,i}$	inhalatory N(L)OAEL for man for endpoint *i*	$[kg_c.m^{-3}]$	S/O
$T25_{mammal,inh,nt}$	inhalatory T25 for mammals for non-threshold effects	$[kg_c.m^{-3}]$	S/O
$CED_{mammal,inh,i}$	inhalatory CED for mammals for endpoint i $i \in$ {repdose,carc,fert,mattox,devtox}	$[kg_c.m^{-3}]$	S/O
$CED_{mammal,inh, nt}$	inhalatory CED for mammals for non-threshold effects	$[kg_c.m^{-3}]$	S/O

Dermal-to-oral route

If dermal and oral absorption rates are known these should be used in the calculations. If these data are not known default values should be taken.

Table III-222 *Defaults for dermal-to-oral extrapolation.*

Parameter	**Symbol** [(a)]	**Unit**	**Value**
Bioavailability for dermal uptake	$BIO_{der,1}$	[-]	
MOLW >500 and [log Kow <-1 or >4]			0.01
MOLW ≤500 and [log Kow ≥-1 and ≤4]			0.1
Bioavailability for oral uptake	$BIO_{oral,2}$	[-]	1

These are parameters are already defined in the sub-modules on human exposure.
(a) “1” indicates starting route, “2” end route.

$$NOAEL_{mammal,oral,i} = NOAEL_{mammal,der,i} \cdot \frac{BIO_{der,1}}{BIO_{oral,2}} \qquad (805)$$

$$LOAEL_{mammal,oral,i} = LOAEL_{mammal,der,i} \cdot \frac{BIO_{der,1}}{BIO_{oral,2}} \qquad (806)$$

$$NOAEL_{man,oral,i} = NOAEL_{man,der,i} \cdot \frac{BIO_{der,1}}{BIO_{oral,2}} \qquad (807)$$

$$LOAEL_{man,oral,i} = LOAEL_{man,der,i} \cdot \frac{BIO_{der,1}}{BIO_{oral,2}} \qquad (808)$$

$$CED_{mammal,oral,i} = CED_{mammal,der,i} \cdot \frac{BIO_{der,1}}{BIO_{oral,2}} \qquad (809)$$

$i \in \{repdose, carc, fert, mattox, devtox\}$

$$T25_{mammal,oral,nt} = T25_{mammal,der,nt} \cdot \frac{BIO_{der,1}}{BIO_{oral,2}} \qquad (810)$$

$$CED_{mammal,oral,nt} = CED_{mammal,der,nt} \cdot \frac{BIO_{der,1}}{BIO_{oral,2}} \qquad (811)$$

If absorption rates of humans and experimental animals differ and are known, the toxicity parameter estimated by EUSES should be corrected manually by multiplication with a factor $BIO_{oral\text{-}animal}/BIO_{oral\text{-}human}$.

Input

$N(L)OAEL_{mammal,der,i}$	dermal N(L)OAEL for mammals for endpoint *i*	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$N(L)OAEL_{man,der,i}$	dermal N(L)OAEL for man for endpoint *i*	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$T25_{mammal,der,nt}$	dermal T25 for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,der,i}$	dermal CED for mammals for endpoint i $i \in$ {repdose,carc,fert,mattox,devtox}	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,der,\ nt}$	dermal CED for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$BIO_{der,1}$	bioavailability for dermal uptake (starting route)	[-]	S/D
$BIO_{oral,2}$	bioavailability for oral uptake (end route)	[-]	S/D

Output

$N(L)OAEL_{mammal,oral,i}$	oral N(L)OAEL for mammals for endpoint *i*	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$N(L)OAEL_{man,oral,i}$	oral N(L)OAEL for man for endpoint *i*	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$T25_{mammal,oral,nt}$	oral T25 for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,oral,i}$	oral CED for mammals for endpoint i $i \in$ {repdose,carc,fert,mattox,devtox}	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,oral,\ nt}$	oral CED for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O

Dermal-to-inhalatory route

If dermal and inhalation absorption rates are known these should be used in the calculations. If these data are not known default values should be taken. The respiratory rate used has to fulfill the requirements of allometric scaling and therefore the inhalatory rate (of humans) is multiplied with the allometric correction factor (AFallom). The TGD proposes the following values: rat 4, mice 7, guinea pig 3, rabbit 2.4, monkey 2, dog 1.4.

Table III-223 *Defaults for dermal-to-inhalation extrapolation.*

Parameter	**Symbol** [(a)]	**Unit**	**Value**
Bioavailability for dermal uptake MOLW >500 and [log Kow <-1 or >4] MOLW ≤500 and [log Kow ≥-1 and ≤4]	$BIO_{der,1}$	[-]	 0.01 0.1
Bioavailability for inhalation	$BIO_{inh,2}$	[-]	1
Body weight of the human considered	BW	$[kg_{bw}]$	70
Daily inhalation rate Consumer / Humans via the environment	IH_{air}	$[m^3.d^{-1}]$	 20

These are parameters are already defined in the sub-modules on human exposure.

(a) “1” indicates starting route, “2” end route.

$$NOAEL_{mammal,inh,i} = NOAEL_{mammal,der,i} \cdot \frac{BW}{IH_{air} \cdot AF_{allom}} \cdot \frac{BIO_{der,1}}{BIO_{inh,2}} \qquad (812)$$

$$LOAEL_{mammal,inh,i} = LOAEL_{mammal,der,i} \cdot \frac{BW}{IH_{air} \cdot AF_{allom}} \cdot \frac{BIO_{der,1}}{BIO_{inh,2}} \qquad (813)$$

$$NOAEL_{man,inh,i} = NOAEL_{man,der,i} \cdot \frac{BW}{IH_{air} \cdot AF_{allom}} \cdot \frac{BIO_{der,1}}{BIO_{inh,2}} \qquad (814)$$

$$LOAEL_{man,inh,i} = LOAEL_{man,der,i} \cdot \frac{BW}{IH_{air} \cdot AF_{allom}} \cdot \frac{BIO_{der,1}}{BIO_{inh,2}} \qquad (815)$$

$$CED_{mammal,inh,i} = CED_{mammal,der,i} \cdot \frac{BW}{IH_{air} \cdot AF_{allom}} \cdot \frac{BIO_{der,1}}{BIO_{inh,2}} \qquad (816)$$

$i \in \{repdose, carc, fert, mattox, devtox\}$

$$T25_{mammal,inh,nt} = T25_{mammal,der,nt} \cdot \frac{BW}{IH_{air} \cdot AF_{allom}} \cdot \frac{BIO_{der,1}}{BIO_{inh,2}} \qquad (817)$$

$$CED_{mammal,inh,nt} = CED_{mammal,der,nt} \cdot \frac{BW}{IH_{air} \cdot AF_{allom}} \cdot \frac{BIO_{der,1}}{BIO_{inh,2}} \qquad (818)$$

If absorption rates of humans and experimental animals differ and are known, the toxicity parameter estimated by EUSES should be corrected manually by multiplication with a factor $BIO_{inh-animal}/BIO_{inh-human}$.

Input

$N(L)OAEL_{mammal,der,i}$	dermal N(L)OAEL for mammals for endpoint *i*	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$N(L)OAEL_{man,der,i}$	dermal N(L)OAEL for man for endpoint *i*	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$T25_{mammal,der,nt}$	dermal T25 for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,der,i}$	dermal CED for mammals for endpoint i $i \in$ {repdose,carc,fert,mattox,devtox}	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,der, nt}$	dermal CED for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$BIO_{der,1}$	bioavailability for dermal uptake (starting route)	[-]	S/D
$BIO_{inh,2}$	bioavailability for inhalation (end route)	[-]	S/D
BW	body weight of the human considered	$[kg_{bw}]$	D
IH_{air}	daily inhalation rate	$[m^3.d^{-1}]$	D
AF_{allom}	allometric scaling factor	[-]	D

Output

$N(L)OAEL_{mammal,inh,i}$	inhalatory N(L)OAEL for mammals for endpoint *i*	$[kg_c.m^{-3}]$	S/O
$N(L)OAEL_{man,inh,i}$	inhalatory N(L)OAEL for man for endpoint *i*	$[kg_c.m^{-3}]$	S/O
$T25_{mammal,inh,nt}$	inhalatory T25 for mammals for non-threshold effects	$[kg_c.m^{-3}]$	S/O
$CED_{mammal,inh,i}$	inhalatory CED for mammals for endpoint i $i \in$ {repdose,carc,fert,mattox,devtox}	$[kg_c.m^{-3}]$	S/O
$CED_{mammal,inh, nt}$	inhalatory CED for mammals for non-threshold effects	$[kg_c.m^{-3}]$	S/O

Inhalatory-to-oral route

If inhalation and oral absorption rates are known these should be used in the calculations. If these data are not known default values should be taken. The respiratory rate used has to fulfill the requirements of allometric scaling and therefore the inhalatory rate (of humans) is multiplied with the allometric correction factor (AFallom). The TGD proposes the following values: rat 4, mice 7, guinea pig 3, rabbit 2.4, monkey 2, dog 1.4.

Table III-224 *Defaults for inhalation-to-oral extrapolation.*

Parameter	**Symbol** (a)	**Unit**	**Value**
Bioavailability for inhalation	$BIO_{inh,1}$	[-]	1
Bioavailability for oral uptake	$BIO_{oral,2}$	[-]	1
Daily inhalation rate Consumer / Humans via the environment	IH_{air}	$[m^3.d^{-1}]$	20
Body weight of the human considered	BW	$[kg_{bw}]$	70

These are parameters are already defined in the sub-modules on human exposure.
(a) “1” indicates starting route, “2” end route.

Input

$N(L)OAEL_{mammal,inh,i}$	inhalatory N(L)OAEL for mammals for endpoint *i*	$[kg_c.m^{-3}]$	S/O
$N(L)OAEL_{man,inh,i}$	inhalatory N(L)OAEL for man for endpoint *i*	$[kg_c.m^{-3}]$	S/O
$T25_{mammal,inh,nt}$	inhalatory T25 for mammals for non-threshold effects	$[kg_c.m^{-3}]$	S/O
$CED_{mammal,inh,i}$	inhalatory CED for mammals for endpoint i $i \in$ {repdose,carc,fert,mattox,devtox}	$[kg_c.m^{-3}]$	S/O
$CED_{mammal,inh,\ nt}$	inhalatory CED for mammals for non-threshold effects	$[kg_c.m^{-3}]$	S/O
$BIO_{inh,1}$	bioavailability for inhalation (starting route)	[-]	S/D
$BIO_{oral,2}$	bioavailability for oral uptake (end route)	[-]	S/D
IH_{air}	daily inhalation rate	$[m^3.d^{-1}]$	D
BW	body weight of the human considered	$[kg_{bw}]$	D
AF_{allom}	allometric scaling factor	[-]	D

Output

$N(L)OAEL_{mammal,oral,i}$	oral N(L)OAEL for mammals for endpoint *i*	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$N(L)OAEL_{man,oral,i}$	oral N(L)OAEL for man for endpoint *i*	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$T25_{mammal,oral,nt}$	oral T25 for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,oral,i}$	oral CED for mammals for endpoint i $i \in$ {repdose,carc,fert,mattox,devtox}	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,oral,\ nt}$	oral CED for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O

$$NOAEL_{mammal,oral,i} = NOAEL_{mammal,inh,i} \cdot \frac{IH_{air} . AF_{allom}}{BW} \cdot \frac{BIO_{inh,1}}{BIO_{oral,2}} \qquad \textbf{(819)}$$

$$LOAEL_{mammal,oral,i} = LOAEL_{mammal,inh,i} \cdot \frac{IH_{air} . AF_{allom}}{BW} \cdot \frac{BIO_{inh,1}}{BIO_{oral,2}} \qquad \textbf{(820)}$$

$$NOAEL_{man,oral,i} = NOAEL_{man,inh,i} \cdot \frac{IH_{air} . AF_{allom}}{BW} \cdot \frac{BIO_{inh,1}}{BIO_{oral,2}} \qquad \textbf{(821)}$$

$$LOAEL_{man,oral,i} = LOAEL_{man,inh,i} \cdot \frac{IH_{air} . AF_{allom}}{BW} \cdot \frac{BIO_{inh,1}}{BIO_{oral,2}} \qquad \textbf{(822)}$$

$$CED_{mammal,oral,i} = CED_{mammal,inh,i} \cdot \frac{IH_{air} . AF_{allom}}{BW} \cdot \frac{BIO_{inh,1}}{BIO_{oral,2}} \qquad \textbf{(823)}$$

$$i \in \{repdose, carc, fert, mattox, devtox\}$$

$$T25_{mammal,oral,nt} = T25_{mammal,inh,nt} \cdot \frac{IH_{air} . AF_{allom}}{BW} \cdot \frac{BIO_{inh,1}}{BIO_{oral,2}} \qquad \textbf{(824)}$$

$$CED_{mammal,oral,nt} = CED_{mammal,inh,nt} \cdot \frac{IH_{air} . AF_{allom}}{BW} \cdot \frac{BIO_{inh,1}}{BIO_{oral,2}} \qquad \textbf{(825)}$$

If absorption rates of humans and experimental animals differ and are known, the toxicity parameter estimated by EUSES should be corrected manually by multiplication with a factor $BIO_{oral\text{-}animal}/BIO_{oral\text{-}human}$.

Inhalatory-to-dermal route

If inhalation and dermal absorption rates are known these should be used in the calculations. If these data are not known default values should be taken. The respiratory rate used has to fulfill the requirements of allometric scaling and therefore the inhalatory rate (of humans) is multiplied with the allometric correction factor (AFallom). The TGD proposes the following values: rat 4, mice 7, guinea pig 3, rabbit 2.4, monkey 2, dog 1.4.

Table III-225 *Defaults for inhalation-to-dermal extrapolation.*

Parameter	**Symbol** (a)	**Unit**	**Value**
Bioavailability for inhalation	$BIO_{inh,1}$	[-]	1
Bioavailability for dermal uptake	$BIO_{der,2}$	[-]	
MOLW >500 and [log Kow <-1 or >4]			0.10
MOLW ≤500 and [log Kow ≥-1 and ≤4]			1
Daily inhalation rate	IH_{air}	$[m^3.d^{-1}]$	
Consumer / Humans via the environment			20
Body weight of the human considered	BW	$[kg_{bw}]$	70

These are parameters are already defined in the sub-modules on human exposure.
(a) “1” indicates starting route, “2” end route.

$$NOAEL_{mammal,der,i} = NOAEL_{mammal,inh,i} \cdot \frac{IH_{air} . AF_{allom}}{BW} \cdot \frac{BIO_{inh,1}}{BIO_{der,2}} \quad \textbf{(826)}$$

$$LOAEL_{mammal,der,i} = LOAEL_{mammal,inh,i} \cdot \frac{IH_{air} . AF_{allom}}{BW} \cdot \frac{BIO_{inh,1}}{BIO_{der,2}} \quad \textbf{(827)}$$

$$NOAEL_{man,der,i} = NOAEL_{man,inh,i} \cdot \frac{IH_{air} . AF_{allom}}{BW} \cdot \frac{BIO_{inh,1}}{BIO_{der,2}} \quad \textbf{(828)}$$

$$LOAEL_{man,der,i} = LOAEL_{man,inh,i} \cdot \frac{IH_{air} . AF_{allom}}{BW} \cdot \frac{BIO_{inh,1}}{BIO_{der,2}} \quad \textbf{(829)}$$

$$CED_{mammal,der,i} = CED_{mammal,inh,i} \cdot \frac{IH_{air} . AF_{allom}}{BW} \cdot \frac{BIO_{inh,1}}{BIO_{der,2}} \quad \textbf{(830)}$$

$$i \in \{repdose, carc, fert, mattox, devtox\}$$

$$T25_{mammal,der,nt} = T25_{mammal,inh,nt} \cdot \frac{IH_{air} . AF_{allom}}{BW} \cdot \frac{BIO_{inh,1}}{BIO_{der,2}} \quad \textbf{(831)}$$

$$CED_{mammal,der,nt} = CED_{mammal,inh,nt} \cdot \frac{IH_{air} . AF_{allom}}{BW} \cdot \frac{BIO_{inh,1}}{BIO_{der,2}} \quad \textbf{(832)}$$

If absorption rates of humans and experimental animals differ and are known, the toxicity parameter estimated by EUSES should be corrected manually by multiplication with a factor $BIO_{der-animal}/BIO_{der-human}$.

Input			
N(L)OAEL$_{mammal,inh,i}$	inhalatory N(L)OAEL for mammals for endpoint *i*	[kg$_c$.m^{-3}]	S/O
N(L)OAEL$_{man,inh,i}$	inhalatory N(L)OAEL for man for endpoint *i*	[kg$_c$.m^{-3}]	S/O
T25$_{mammal,inh,nt}$	inhalatory T25 for mammals for non-threshold effects	[kg$_c$.m^{-3}]	S/O
CED$_{mammal,inh,i}$	inhalatory CED for mammals for endpoint i	[kg$_c$.m^{-3}]	S/O
	$i \in$ {repdose,carc,fert,mattox,devtox}		
CED$_{mammal,inh, nt}$	inhalatory CED for mammals for non-threshold effects	[kg$_c$.m^{-3}]	S/O
BIO$_{inh,1}$	bioavailability for inhalation (starting route)	[-]	S/D
BIO$_{der,2}$	bioavailability for dermal uptake (end route)	[-]	S/D
IH$_{air}$	daily inhalation rate	[m^3.d^{-1}]	D
BW	body weight of the human considered	[kg$_{bw}$]	D
AF$_{allom}$	allometric scaling factor	[-]	D
Output			
N(L)OAEL$_{mammal,der,i}$	dermal N(L)OAEL for mammals for endpoint *i*	[kg$_c$.kg$_{bw}$$^{-1}$.d^{-1}]	S/O
N(L)OAEL$_{man,der,i}$	dermal N(L)OAEL for man for endpoint *i*	[kg$_c$.kg$_{bw}$$^{-1}$.d^{-1}]	S/O
	$i \in$ {repdose,carc,fert,mattox,devtox}		
T25$_{mammal,der,nt}$	dermal T25 for mammals for non-threshold effects	[kg$_c$.kg$_{bw}$$^{-1}$.d^{-1}]	S/O
CED$_{mammal,der,i}$	dermal CED for mammals for endpoint i	[kg$_c$.kg$_{bw}$$^{-1}$.d^{-1}]	S/O
	$i \in$ {repdose,carc,fert,mattox,devtox}		
CED$_{mammal,der, nt}$	dermal CED for mammals for non-threshold effects	[kg$_c$.kg$_{bw}$$^{-1}$.d^{-1}]	S/O

For the route-to-route extrapolation for workers involving the inhalatory route an additional correction is used to account for the difference between the respiratory rate of the general population (default 20 m3 per 24 hrs), used in the route-to-route extrapolation, and the respiratory rate of workers (10 m3 in 8 hrs). The TGD recommends a factor of 0.5 for extrapolations from the dermal and oral route to the inhalatory route and 2 for extrapolations from the inhalatory route to the dermal and oral route. EUSES allows this correction in the derivation of the RMOS, RMOE and human equivalent dose for workers. The default is 1.

III.6.2.2 Conversion from mg.kg$_{food}$$^{-1}$(diet studies) to mg.kg$_{bw}$$^{-1}$.d^{-1}

If NOAEL is absent and NOEC is available:

$$NOAEL_{mammal,oral,chr} = \frac{NOEC_{mammal,\ food,chr}}{CONV_{mammal}} \qquad \textbf{(833)}$$

If LOAEL is absent and LOEC is available:

$$LOAEL_{mammal,oral,chr} = \frac{LOEC_{mammal,\ food,chr}}{CONV_{mammal}} \qquad \textbf{(834)}$$

If T25 is only available from a diet study in mg/kg food:

$$T25_{mammal,oral,nt} = \frac{T25_{mammal,\ food,nt}}{CONV_{mammal}} \qquad \textbf{(835)}$$

If CED is only available from a diet study in mg/kg food:

$$CED_{mammal,oral,nt} = \frac{CED_{mammal,\ food,nt}}{CONV_{mammal}} \qquad \textbf{(836)}$$

$$i \in \{repdose, carc,\ fert, mattox, devtox\}$$

Input

$N(L)OEC_{mammal,food,i}$	N(L)OEC via food for mammals for endpoint *i*	$[kg_c.kg_{food}^{-1}]$	S/O
$T25_{mammal,food,nt}$	T25 via food for mammals for non-threshold substances	$[kg_c.kg_{food}^{-1}]$	S/O
$CED_{mammal,food,i}$	CED via food for mammals for endpoint i	$[kg_c.kg_{food}^{-1}]$	S/O
$CED_{mammal,food,nt}$	CED via food for mammals for non-threshold substances	$[kg_c.kg_{food}^{-1}]$	S/O
$CONV_{mammal}$	conversion factor NOAEL to NOEC	$[kg_{bw}.d.kg_{food}^{-1}]$	P/S [a]
	$i \in$ {repdose,carc,fert,mattox,devtox}		

Output

$N(L)OAEL_{mammal,oral,i}$	oral N(L)OAEL for mammals for endpoint *i*	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$T25_{mammal,oral,nt}$	oral T25 for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,oral,i}$	oral CED for mammals for endpoint i	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
	$i \in$ {repdose,carc,fert,mattox,devtox}		
$CED_{mammal,oral,\ nt}$	oral CED for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O

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[a] see Table III-219 in Section III.6.1.5.

III.7 RISK CHARACTERISATION

In risk characterisation, exposure levels are compared to suitable no-effect levels to yield so-called Risk Characterisation Ratios (RCR) for each protection goal. For the environmental end-points, this is the ratio of PEC to PNEC. For the human end-points a distinction need to be made between threshold and non-threshold substances. For threshold substances the Margin Of Safety (MOS) is derived, i.e. the ratio of the effect parameter and the estimated exposure value. The MOS is compared to a reference-MOS. In addition, for biocides the Acceptable-Operator-Exposure-Level (AOEL) is compared to the internal exposure value. Risk characterisation of non-threshold substances entails a comparison between the estimated exposure and the T25 or BMD05, extrapolated to a lifetime cancer risk for humans. Additionally, the Margin of Exposure (MOE) approach is followed. This approach is equivalent to the MOS approach for threshold substances: the MOE is the ratio of the effect parameter (T25 or BMD05) and the estimated lifetime daily exposure level. The MOE is to be compared to the reference-MOE.. Environmental risk characterisation and human health risk characterisation are handled in separate sub-modules.

This module is divided into four specific sub-modules, which will be treated separately:

- Environment.
- Indirect human exposure.
- Consumer exposure.
- Workplace exposure.

III.7.1 Risk characterisation for the environment

Input

PEClocal$_{water}$	local PEC in surface water during emission episode	[kg$_c$.m^{-3}]	
PEClocal$_{water,marine}$	local PEC in marine surface water during emission episode	[kg$_c$.m^{-3}]	
PECreg$_{water}$	regional steady-state PEC in surface water	[kg$_c$.m^{-3}]	
PECreg$_{water,marine}$	regional steady-state PEC in marine surface water	[kg$_c$.m^{-3}]	
PNEC$_{water}$	PNEC for the aquatic compartment	[kg$_c$.m^{-3}]	c
PNEC$_{water,marine}$	PNEC for the marine aquatic compartment	[kg$_c$.m^{-3}]	c
PEClocal$_{soil}$	local PEC in agricultural soil, averaged over 30 days	[kg$_c$.kg$_{wwt}^{-1}$]	
PECreg$_{agric}$	regional steady-state PEC in agricultural soil	[kg$_c$.kg$_{wwt}^{-1}$]	
PNEC$_{soil}$	PNEC for the soil compartment	[kg$_c$.kg$_{wwt}^{-1}$]	c
TOXterr	toxicological data used for extrapolation of PNEC	[kg$_c$.kg$_{wwt}^{-1}$]	
EPterr	equilibrium partitioning used for PNEC for soil?	[yes/no]	c
Kow	octanol-water partition coefficient	[m^3.m^{-3}]	
PEClocal$_{sed}$	local PEC in sediment	[kg$_c$.kg$_{wwt}^{-1}$]	
PEClocal$_{sed,marine}$	local PEC in marine sediment	[kg$_c$.kg$_{wwt}^{-1}$]	
PECreg$_{sed}$	regional steady-state PEC in sediment	[kg$_c$.kg$_{wwt}^{-1}$]	
PECreg$_{sed,marine}$	regional steady-state PEC in marine sediment	[kg$_c$.kg$_{wwt}^{-1}$]	
PNEC$_{sed}$	PNEC for the sediment compartment	[kg$_c$.kg$_{wwt}^{-1}$]	
PNEC$_{sed,marine}$	PNEC for the marine sediment compartment	[kg$_c$.kg$_{wwt}^{-1}$]	
EPsed	equilibrium partitioning used for PNEC for sediment?	[yes/no]	c
EPsed$_{marine}$	equilibrium partitioning used for PNEC for marine sediment?	[yes/no]	c
PEC$_{stp}$	local PEC in STP during emission episode	[kg$_c$.m^{-3}]	
PNEC$_{micro-organisms}$	PNEC for STP micro-organisms	[kg$_c$.m^{-3}]	c
PEC$_{oral,fish}$	PEC in fish (local and regional combined)	[kg$_c$.kg$_{wwt}^{-1}$]	
PEC$_{oral,fish,marine}$	PEC in marine fish (local and regional combined)	[kg$_c$.kg$_{wwt}^{-1}$]	
PEC$_{oral,fish\ predator,marine}$	PEC in marine fish-eating predator (local and regional combined)	[kg$_c$.kg$_{wwt}^{-1}$]	
PEC$_{oral,worm}$	PEC in worm (local and regional combined)	[kg$_c$.kg$_{wwt}^{-1}$]	
PNEC$_{oral}$	PNEC for birds and mammals	[kg$_c$.kg$_{wwt}^{-1}$]	c
PNECstat$_{water}$	PNEC for aquatic organisms with statistical method	[kg$_c$.m^{-3}]	
PNECstat$_{water,\ marine}$	PNEC for marine aquatic organisms with statistical method	[kg$_c$.m^{-3}]	
PNECstat$_{soil}$	PNEC for terrestrial organisms with statistical method	[kg$_c$.m^{-3}]	

Output

RCRlocal$_{water}$	RCR for the local water compartment	[-]	c
RCRlocal$_{water,marine}$	RCR for the local marine water compartment	[-]	c
RCRreg$_{water}$	RCR for the regional water compartment	[-]	c
RCRreg$_{water,marine}$	RCR for the regional marine water compartment	[-]	c
RCRlocal$_{soil}$	RCR for the local soil compartment	[-]	c
RCRreg$_{soil}$	RCR for the regional soil compartment	[-]	c
RCRlocal$_{sed}$	RCR for the local sediment compartment	[-]	c
RCRlocal$_{sed,marine}$	RCR for the local marine sediment compartment	[-]	c
RCRreg$_{sed}$	RCR for the regional sediment compartment	[-]	c
RCRreg$_{sed,marine}$	RCR for the regional marine sediment compartment	[-]	c
RCR$_{stp}$	RCR for the sewage treatment plant	[-]	c
RCR$_{oral,fish}$	RCR for fish-eating birds and mammals	[-]	c
RCR$_{oral,fish,marine}$	RCR for fish-eating birds/mammals (marine environment)	[-]	c
RCR$_{oral,fish\ predator,marine}$	RCR for top-predators (marine environment)	[-]	c
RCR$_{oral,worm}$	RCR for worm-eating birds and mammals	[-]	c
RCRstat$_{water}$	RCR for aquatic organisms with statistical method	[-]	c
RCRstat$_{water,\ marine}$	RCR for marine aquatic organisms with statistical method	[-]	c
RCRstat$_{soil}$	RCR for terrestrial organisms with statistical method	[-]	c

III.7.1.1 Aquatic environment

The concentration of the chemical in surface water is compared to the no-effect concentration for aquatic organisms. This is done for the local as well as the regional freshwater and marine environment. On the local scale, the concentration during an emission episode is taken. It should be noted that the local ratios have to be defined for all relevant stages of the life cycle and for each application of the substance.

$$RCRlocal_{water} = \frac{PEClocal_{water}}{PNEC_{water}} \tag{837}$$

$$RCRlocal_{water,marine} = \frac{PEClocal_{water,marine}}{PNEC_{water,marine}} \tag{838}$$

$$RCRreg_{water} = \frac{PECreg_{water}}{PNEC_{water}} \tag{839}$$

$$RCRreg_{water,marine} = \frac{PECreg_{water,marine}}{PNEC_{water,marine}} \tag{840}$$

Input			
$PEClocal_{water}$	local PEC in surface water during emission episode	$[kg_c.m^{-3}]$	O
$PECreg_{water}$	regional steady-state PEC in surface water	$[kg_c.m^{-3}]$	O
$PEClocal_{water,marine}$	local PEC in marine water during emission episode	$[kg_c.m^{-3}]$	O
$PECreg_{water,marine}$	regional steady-state PEC in marine surface water	$[kg_c.m^{-3}]$	O
$PNEC_{water}$	PNEC for aquatic compartment	$[kg_c.m^{-3}]$	O^c
$PNEC_{water,marine}$	PNEC for marine aquatic compartment	$[kg_c.m^{-3}]$	O^c
Output			
$RCRlocal_{water}$	RCR for local water compartment	[-]	O^c
$RCRreg_{water}$	RCR for regional water compartment	[-]	O^c
$RCRlocal_{water,marine}$	RCR for local marine water compartment	[-]	O^c
$RCRreg_{water,marine}$	RCR for regional marine water compartment	[-]	O^c

III.7.1.2 Terrestrial compartment

The concentration of the chemical in agricultural soil is compared to the no-effect concentration for terrestrial organisms. This is done for the local as well as the regional environment. On the local scale, the concentration averaged over 30 days is used. It should be noted that the local ratios have to be defined for all relevant stages of the life cycle and for each application of the substance. For substances with a log *Kow* greater than 5, the equilibrium-partitioning method is used in a modified way. For these substances, the PEC/PNEC in soil is increased by a factor of 10 to account for uptake via ingestion of soil.

$$RCRlocal_{soil} = \frac{PEClocal_{soil}}{PNEC_{soil}} \tag{841}$$

$$RCRreg_{soil} = \frac{PECreg_{agric}}{PNEC_{soil}} \tag{842}$$

If *EPterr* = yes and log *Kow* > 5 then

$$RCRlocal_{soil} = \frac{PEClocal_{soil}}{PNEC_{soil}} \cdot 10 \tag{843}$$

If *EPterr* = yes and log *Kow* > 5 then

$$RCRreg_{soil} = \frac{PECreg_{agric}}{PNEC_{soil}} \cdot 10 \tag{844}$$

Input			
$PEClocal_{soil}$	local PEC in agricultural soil, averaged over 30 days	$[kg_c.kg_{wwt}^{-1}]$	O
$PECreg_{agric}$	regional steady-state PEC in agricultural soil	$[kg_c.kg_{wwt}^{-1}]$	O
$PNEC_{soil}$	PNEC for soil compartment	$[kg_c.kg_{wwt}^{-1}]$	O^c
EPterr	equilibrium partitioning used for PNEC?	[yes/no]	O^c
Kow	octanol-water partition coefficient	$[m^3.m^{-3}]$	S
Output			
$RCRlocal_{soil}$	RCR for local soil compartment	[-]	O^c
$RCRreg_{soil}$	RCR for regional soil compartment	[-]	O^c

III.7.1.3 Sediment compartment

The concentration of the chemical in sediment is compared to the no-effect concentration for sediment-dwelling organisms. This is done for the local as well as the regional freshwater and marine environment. It should be noted that the local ratios have to be defined for all relevant stages of the life cycle and for each application of the substance. For substances with a log *Kow* greater than 5, the equilibrium-partitioning method is used in a modified way. For these substances, the PEC/PNEC in sediment is increased by a factor of 10 to account for uptake via ingestion of sediment. It should be noted that a risk characterisation for sediment is only feasible if measured data are used to overwrite the estimates for PEC and/or PNEC in sediment (otherwise, equilibrium partitioning is applied to derive both PEC and PNEC).

$$RCRlocal_{sed} = \frac{PEClocal_{sed}}{PNEC_{sed}} \tag{845}$$

$$RCRlocal_{sed,marine} = \frac{PEClocal_{sed,marine}}{PNEC_{sed,marine}} \tag{846}$$

$$RCRreg_{sed} = \frac{PECreg_{sed}}{PNEC_{sed}} \tag{847}$$

$$RCRreg_{sed,marine} = \frac{PECreg_{sed,marine}}{PNEC_{sed,marine}} \tag{848}$$

If *EPsed* = yes and log *Kow* > 5 then:

$$RCRlocal_{sed} = \frac{PEClocal_{sed}}{PNEC_{sed}} \cdot 10 \tag{849}$$

$$RCRreg_{sed} = \frac{PECreg_{sed}}{PNEC_{sed}} \cdot 10 \tag{850}$$

If $EPsed_{marine}$ = yes and log *Kow* > 5 then:

$$RCRlocal_{sed,marine} = \frac{PEClocal_{sed,marine}}{PNEC_{sed,marine}} \cdot 10 \tag{851}$$

$$RCRreg_{sed,marine} = \frac{PECreg_{sed,marine}}{PNEC_{sed,marine}} \cdot 10 \tag{852}$$

Input			
$PEClocal_{sed}$	local PEC in sediment	$[kg_c.kg_{wwt}^{-1}]$	O
$PEClocal_{sed,marine}$	local PEC in marine sediment	$[kg_c.kg_{wwt}^{-1}]$	O
$PECreg_{sed}$	regional steady-state PEC in sediment	$[kg_c.kg_{wwt}^{-1}]$	O
$PECreg_{sed,marine}$	regional steady-state PEC in marien sediment	$[kg_c.kg_{wwt}^{-1}]$	O
$PNEC_{sed}$	PNEC for the sediment compartment	$[kg_c.kg_{wwt}^{-1}]$	O
$PNEC_{sed,marine}$	PNEC for the marine sediment compartment	$[kg_c.kg_{wwt}^{-1}]$	O
EPsed	equilibrium partitioning used for PNEC for sediment?	[yes/no]	O^c
$EPsed_{marine}$	equilibrium partitioning used for PNEC for marine sediment?	[yes/no]	O^c
Kow	octanol-water partition coefficient	$[m^3.m^{-3}]$	S
Output			
$RCRlocal_{sed}$	RCR for local sediment compartment	[-]	O^c
$RCRlocal_{sed,marine}$	RCR for local marine sediment compartment	[-]	O^c
$RCRreg_{sed}$	RCR for regional sediment compartment	[-]	O^c
$RCRreg_{sed,marine}$	RCR for regional marine sediment compartment	[-]	O^c

III.7.1.4 Micro-organisms in STP

The concentration of the chemical in the sewage treatment plant is compared to the no-effect concentration for micro-organisms. This is done for the local environment only. The concentration during an emission episode is used. It should be noted that the ratios have to be defined for all relevant stages of the life cycle and for each application of the substance.

$$RCR_{stp} = \frac{PEC_{stp}}{PNEC_{micro\text{-}organisms}} \tag{853}$$

Input			
PEC_{stp}	local PEC in STP during emission episode	$[kg_c.m^{-3}]$	O
$PNEC_{micro\text{-}organisms}$	PNEC for STP micro-organisms	$[kg_c.m^{-3}]$	O^c
Output			
RCR_{stp}	RCR for sewage treatment plant	[-]	O^c

III.7.1.5 Predators in freshwater and marine environment

The concentration of the chemical in fish and in fish-eating predator is compared to the no-effect concentration for birds and mammals. Local and regional concentrations are combined for calculating the concentration in fish and fish-eating predator . It should be noted that the ratios have to be defined for all relevant stages of the life cycle and for each application of the substance.

$$RCR_{oral,fish} = \frac{PEC_{oral,fish}}{PNEC_{oral}} \tag{854}$$

$$RCR_{oral,fish,marine} = \frac{PEC_{oral,fish,marine}}{PNEC_{oral}} \tag{855}$$

$$RCR_{oral,\ fish\ predator,marine} = \frac{PEC_{oral,\ fish\ predator,marine}}{PNEC_{oral}} \tag{856}$$

put			
$PEC_{oral,fish}$	PEC in fish (local and regional combined)	$[kg_{c}.kg_{wwt}^{-1}]$	O
$PEC_{oral,fish,marine}$	PEC in marine fish (local and regional combined)	$[kg_{c}.kg_{wwt}^{-1}]$	O
$PEC_{oral,fish\ predator,marine}$	PEC in marine fish-eating predator (local and regional combined)	$[kg_{c}.kg_{wwt}^{-1}]$	O
$PNEC_{oral}$	PNEC for birds and mammals	$[kg_{c}.kg_{wwt}^{-1}]$	O^{c}
Output			
$RCR_{oral,fish}$	RCR for fish-eating birds/mammals (freshwater environment)	[-]	O^{c}
$RCR_{oral,fish,marine}$	RCR for fish-eating birds/mammals (marine environment)	[-]	O^{c}
$RCR_{oral,fish\ predator,marine}$	RCR for top-predators (marine environment)	[-]	O^{c}

III.7.1.6 Worm-eating predators

The concentration of the chemical in earthworms is compared to the no-effect concentration for birds and mammals. There is only one concentration in earthworms as local and regional are combined in this concentration. It should be noted that the ratios have to be defined for all relevant stages of the life cycle and for each application of the substance.

$$RCR_{oral,worm} = \frac{PEC_{oral,worm}}{PNEC_{oral}} \tag{857}$$

Input			
$PEC_{oral,worm}$	PEC in worm (local and regional combined)	$[kg_{c}.kg_{wwt}^{-1}]$	O
$PNEC_{oral}$	PNEC for birds and mammals	$[kg_{c}.kg_{wwt}^{-1}]$	O^{c}
Output			
$RCR_{oral,worm}$	RCR for worm-eating birds and mammals	[-]	O^{c}

III.7.2 Risk characterisation for human health

For threshold-based effects, the quantitative risk characterisation is carried out by calculating 'Margins Of Safety' (MOS) and comparing this to a reference-MOS (MOS approach). This MOS approach is not applicable for non-threshold based effects. Next to the MOS approach, **for biocides** an Acceptable Operator Exposure Level (AOEL) is to be derived, which should be compared to the estimated exposure values. For non-threshold effects, i.e. genotoxic carcinogens, lifetime cancer risk is calculated based on T25 or CED05. Additionally, the Margin of Exposure (MOE) is calculated and compared to a reference-MOE (RMOE).

Table III-226 *Defaults factors*

Assessment factor	**Symbol**	**Unit**	**Value**
Allometric scaling factor	AF_{allom}	[-]	1[a]
Remaining interspecies differences	AF_{inter}	[-]	1[b]
Intraspecies differences	AF_{intra}	[-]	1[c]
Differences in exposure duration	AF_{expdur}	[-]	1[d]
Differences in exposure route	AF_{exprt}	[-]	1[e]
Dose-response relationship	$AF_{dose-resp}$	[-]	1[f]
Low risk extrapolation factor	AF_{lr}	[-]	250,000[g]
Correction factors workers			
Correction factor for route-to route extrapolation to account for difference in ventilation rate between workers and general population	CF_{occup1}	[-]	1[h]
Correction factor for duration and frequency of exposure	CF_{occup2}	[-]	2.8

[a] Correction for differences in metabolic size: the TGD recommends 4 for rats, 7 for mice, 3 for guinea pigs, 2.4 for rabbits, 2 for monkeys and 1.4 for dogs

[b] The TGD recommends 2.5

[c] The TGD recommends 5 for workers and 10 for the general population

[d] The TGD recommends 3 for subacute to sub/semi-chronic extrapolation, 2 for sub/semi-chronic to chronic extrapolation amd 6 for subacute to chronic extrapolation

[e] Factor to account for uncertainty in the route-to-route extrapolation

[f] Factor to account for uncertainty in the dose-response extrapolation; includes uncertainty regarding the nature of the effect and the quality of the database

[g] Factor, used for the calculation of the reference-MOE for non-threshold substances, accounting for the extrapolation for the high risk related to the T25 (25:100) to a low reference level, default chosen to be $1:10^6$

[h] Factor accounting for the difference between the respiratory rate of the general population (default 20 m^3 per 24 hrs) used in the route-to-route extrapolation and the respiratory rate of workers (10 m^3 in 8 hrs). The TGD recommends a factor of 0.5 for extrapolations from the dermal and oral route to the inhalatory route and 2 for extrapolations from the inhalatory route to the dermal and oral route.

III.7.2.1 Risk characterisation for humans exposed via the environment

III.7.2.1.1 Threshold substances

Calculation of scenario-specific MOS

Under the assumption that man is exposed throughout his or her lifetime, the total daily intake of a substance in food, drinking water and air is compared to the oral N(L)OAEL from repeated dose toxicity studies, carcinogenicity studies (unless carcinogenicity is via a non-threshold mode of action) and/or reproductive toxicity studies, resulting in a Risk Characterisation Ratio (RCR) called the Margin Of Safety, MOS. This comparison is made for both the local and the regional scale. If both an N(L)OAEL for man and an N(L)OAEL for mammals are available, the former one is used in this risk characterisation. In addition, the air concentration estimated for man in the standard environment is compared to the inhalatory N(L)OAEL for these endpoints.

Depending on the available data the following RCRs are possible:

Effects / Exposure	**Exposure**	**Available effects data**
$MOSman\text{-}env_{local,tot,i}$	$DOSElocal_{tot}$	$NOAEL_{mammal,oral,i}$ $LOAEL_{mammal,oral,i}$ $NOAEL_{man,oral,i}$ $LOAEL_{man,oral,i}$ $CED_{mammal,oral,i}$
$MOSman\text{-}env_{reg,tot,i}$	$DOSEreg_{tot}$	$NOAEL_{mammal,oral,i}$ $LOAEL_{mammal,oral,i}$ $NOAEL_{man,oral,i}$ $LOAEL_{man,oral,i}$ $CED_{mammal,oral,i}$
$MOSman\text{-}env_{local,inh,i}$	$PEClocal_{air,ann}$	$NOAEL_{mammal,inh,i}$ $LOAEL_{mammal,inh,i}$ $NOAEL_{man,inh,i}$ $LOAEL_{man,inh,i}$ $CED_{mammal,inh,i}$
$MOSman\text{-}env_{reg,inh,i}$	$PECreg_{air}$	$NOAEL_{mammal,inh,i}$ $LOAEL_{mammal,inh,i}$ $NOAEL_{man,inh,i}$ $LOAEL_{man,inh,i}$ $CED_{mammal,inh,i}$

$i \in \{repdose,carc,fert,mattox,devtox\}$

Input

$N(L)OAEL_{mammal,oral,i}$	oral N(L)OAEL for mammals for endpoint of concern	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$N(L)OAEL_{man,oral,i}$	oral N(L)OAEL for man for endpoint of concern	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$N(L)OAEL_{mammal,inh,i}$	inhalatory N(L)OAEL for mammals for endpoint of concern	$[kg_c.m^{-3}]$	S/O
$N(L)OAEL_{man,inh,i}$	inhalatory N(L)OAEL for man for endpoint of concern	$[kg_c.m^{-3}]$	S/O
$CED_{mammal,oral,i}$	oral CED for mammals for endpoint of concern	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S
$CED_{mammal,inh,i}$	inhalatory CED for mammals for endpoint of concern	$[kg_c.m^{-3}]$	S
$DOSElocal_{tot}$	local total daily intake for humans	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$DOSEreg_{tot}$	regional total daily intake for humans	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$PEClocal_{air,ann}$	annual average local PEC in air (total)	$[kg_c.m^{-3}]$	O
$PECreg_{air}$	regional PEC in air (total)	$[kg_c.m^{-3}]$	O
	$i \in$ {repdose,carc,fert,mattox,devtox}		

Output

$MOSman\text{-}env_{local,tot,i}$	MOS local, total exposure via all media, for endpoint of concern	[-]	O^c
$MOSman\text{-}env_{local,inh,i}$	MOS local, exposure via air, for endpoint of concern	[-]	O^c
$MOSman\text{-}env_{reg,tot,i}$	MOS regional, total exposure via all media, for endpoint of conc.	[-]	O^c
$MOSman\text{-}env_{reg,inh,i}$	MOS regional, exposure via air, for endpoint of concern	[-]	O^c
	$i \in$ {repdose,carc,fert,mattox,devtox}		

Derivation of scenario-specific reference-MOS

In order to account for the various uncertainties and variabilities in the extrapolation from experimental data to the human situation and in the available data set, per scenario under consideration a reference-MOS is to be derived. All aspects that can be dealt with quantitatively (as assessment factors) are combined to form the overall assessment factor or reference-MOS (RMOS).

$$RMOSman - env_{x,y,i} = AF_{inter} \cdot AF_{allom} \cdot AF_{intra} \cdot AF_{expdur} \cdot AF_{exprt} \cdot AF_{dose-resp} \tag{858}$$

$x \in$ {local,reg}
$y \in$ {tot,inh}
$i \in$ {repdose,carc,fert,mattox,devtox}

Input

AF_{allom}	assessment factor for allometric scaling	[-]	S/D
AF_{inter}	assessment factor for remaining interspecies differences	[-]	S/D
AF_{intra}	assessment factor for intraspecies differences	[-]	S/D
AF_{expdur}	assessment factor for differences in exposure duration	[-]	S/D
AF_{exprt}	assessment factor for differences in exposure route	[-]	S/D
$AF_{dose-resp}$	assessment factor for dose-response relationship	[-]	S/D

Output

$RMOSman\text{-}env_{local,tot,i}$	reference-MOS local, total exposure via all media, for endpoint of concern	[-]	O^c
$RMOSman\text{-}env_{local,inh,i}$	reference-MOS local, exposure via air, for endpoint of concern	[-]	O^c
$RMOSman\text{-}env_{reg,tot,i}$	reference-MOS regional, total exposure via all media, for endpoint of concern	[-]	O^c
$RMOSman\text{-}env_{reg.inh,i}$	reference-MOS regional, exposure via air, for endpoint of concern	[-]	O^c
	$i \in$ {repdose,carc,fert,mattox,devtox}		

Comparison of MOS with reference-MOS

In judging the acceptability of the MOS, in a second step of the quantitative risk characterisation the MOS is compared to the reference-MOS, resulting in a MOS/reference-MOS ratio (MRR).

Depending on the available data the following MRRs are possible:

RCR / reference-MOS	**RCR**	**Reference-MOS**
$MRRman\text{-}env_{local,tot,i}$	$MOSman\text{-}env_{local,tot,i}$	$RMOSman\text{-}env_{local,tot,i}$
$MRRman\text{-}env_{reg,tot,i}$	$MOSman\text{-}env_{reg,tot,i}$	$RMOSman\text{-}env_{reg,tot,i}$
$MRRman\text{-}env_{local,inh,i}$	$MOSman\text{-}env_{local,inh,i}$	$RMOSman\text{-}env_{local,inh,i}$
$MRRman\text{-}env_{reg,inh,i}$	$MOSman\text{-}env_{reg,inh,i}$	$RMOSman\text{-}env_{reg,inh,i}$

$i \in$ {repdose,carc,fert,mattox,devtox}

Input

$MOSman\text{-}env_{local,tot,i}$	MOS local, total exposure via all media, for endpoint of concern	[-]	O^c
$MOSman\text{-}env_{local,inh,i}$	MOS local, exposure via air, for endpoint of concern	[-]	O^c
$MOSman\text{-}env_{reg,tot,i}$	MOS regional, total exposure via all media, for endpoint of conc.	[-]	O^c
$MOSman\text{-}env_{reg,inh,i}$	MOS regional, exposure via air, for endpoint of concern	[-]	O^c
$RMOSman\text{-}env_{local,tot,i}$	reference-MOS local, total exposure via all media, for endpoint of concern	[-]	O^c
$RMOSman\text{-}env_{local,inh,i}$	reference-MOS local, exposure via air, for endpoint of concern	[-]	O^c
$RMOSman\text{-}env_{reg,tot,i}$	reference-MOS regional, total exposure via all media, for endpoint of concern	[-]	O^c
$RMOSman\text{-}env_{reg.inh,i}$	reference-MOS regional, exposure via air, for endpoint of concern	[-]	O^c
	$i \in$ {repdose,carc,fert,mattox,devtox}		

Output

$MRRman\text{-}env_{local,tot,i}$	ratio MOS/reference-MOS local, total exposure via all media, for endp. of concern	[-]	O^c
$MRRman\text{-}env_{local,inh,i}$	ratio MOS/reference-MOS local, exposure via air, for endpoint of concern	[-]	O^c
$MRRman\text{-}env_{reg,tot,i}$	ratio MOS/reference-MOS regional, total exposure via all media, for endp. of conc.	[-]	O^c
$MRRman\text{-}env_{reg.inh,i}$	ratio MOS/reference-MOS regional, exposure via air, for endpoint of concern	[-]	O^c
	$i \in$ {repdose,carc,fert,mattox,devtox}		

III.7.2.1.2 Non-threshold substances

A. Lifetime carcinogenic risk

Starting point is the T25 which first needs to be converted to an equivalent human dose descriptor, the HT25, applying allometric assessment factors and, possibly, an assessment factor for route-to-route extrapolation.

$$AFman-env_{x,y,nt} = AF_{allom} \cdot AF_{\exp rt}$$

$x \in$ {local,reg}

$y \in$ {tot,inh}

Input

AF_{allom}	assessment factor for allometric scaling	[-]	S/D
AF_{exprt}	assessment factor for differences in exposure route	[-]	S/D

Output

$AFman\text{-}env_{local,tot,nt}$	assessment factor local, exposure via all media, non-thr.	[-]	S/O
$AFman\text{-}env_{reg,tot,nt}$	assessment factor regional, exposure via all media, non-thr.	[-]	S/O
$AFman\text{-}env_{local,inh,nt}$	assessment factor local, exposure via air, non-thr.	[-]	S/O
$AFman\text{-}env_{local,inh,nt}$	assessment factor regioanl, exposure via air, non-thr.	[-]	S/O

$$HT25man-env_{x,tot,nt} = \frac{T25_{mammal,oral,nt}}{AFman-env_{x,tot,nt}} \quad \textbf{(859)}$$

$$HT25man-env_{x,inh,nt} = \frac{T25_{mammal,inh,nt}}{AFman-env_{x,inh,nt}} \quad \textbf{(860)}$$

$x \in$ {local,reg}

Input

$T25_{mammal,oral,nt}$	oral T25 for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$T25_{mammal,inh,nt}$	inhalatory T25 for mammals for non-threshold effects	$[kg_c.m^{-3}]$	S/O
$AFman\text{-}env_{local,tot,nt}$	assessment factor local, exposure via all media, non-thr.	[-]	S/O
$AFman\text{-}env_{reg,tot,nt}$	assessment factor regional, exposure via all media, non-thr.	[-]	S/O
$AFman\text{-}env_{local,inh,nt}$	assessment factor local, exposure via air, non-thr.	[-]	S/O
$AFman\text{-}env_{local,inh,nt}$	assessment factor regioanl, exposure via air, non-thr.	[-]	S/O

Output

$HT25man\text{-}env_{local,tot,nt}$	human equivalent dose local, exposure via all media, non-thr.	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$HT25man\text{-}env_{reg,tot,nt}$	human equivalent dose regional, exposure via all media, non-thr.	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$HT25man\text{-}env_{local,inh,nt}$	human equivalent dose local, exposure via air media, non-thr.	$[kg_c.m^{-3}]$	O
$HT25man\text{-}env_{reg,inh,nt}$	human equivalent dose regional, exposure via air media, non-thr.	$kg_c.m^{-3}]$	O

Subsequently the lifetime cancer risk is calculated for total exposure to and inhalation of ambient air at each spatial scale.

$$cLRman-env_{local,tot,nt} = \frac{DOSElocal_{tot}}{HT25man-env_{local,tot,nt}} \cdot 0.25 \quad \textbf{(861)}$$

$$cLRman-env_{reg,tot,nt} = \frac{DOSEreg_{tot}}{HT25man-env_{reg,tot,nt}} \cdot 0.25 \quad \textbf{(862)}$$

$$cLRman-env_{local,inh,nt} = \frac{PEClocal_{air,ann}}{HT25man-env_{local,inh,nt}} \cdot 0.25 \quad \textbf{(863)}$$

$$cLRman-env_{reg,inh,nt} = \frac{PECreg_{air}}{HT25man-env_{reg,inh,nt}} \cdot 0.25 \quad \textbf{(864)}$$

Input

$DOSElocal_{tot}$	local total daily intake for humans	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$DOSEreg_{tot}$	regional total daily intake for humans	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$PEClocal_{air,ann}$	annual average local PEC in air (total)	$[kg_c.m^{-3}]$	O
$PECreg_{air}$	regional PEC in air (total)	$[kg_c.m^{-3}]$	O
$HT25man\text{-}env_{local,tot,nt}$	human equivalent dose local, exposure via all media, non-thr.	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$HT25man\text{-}env_{reg,tot,nt}$	human equivalent dose regional, exposure via all media, non-thr.	$kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$HT25man\text{-}env_{local,inh,nt}$	human equivalent dose local, exposure via air media, non-thr.	$[kg_c.m^{-3}]$	O
$HT25man\text{-}env_{reg,inh,nt}$	human equivalent dose regional, exposure via air media, non-thr.	$[kg_c.m^{-3}]$	O

Output

$cLRman\text{-}env_{local,tot,nt}$	lifetime cancer risk local, exposure via all media, non-thr.	[-]	O
$cLRman\text{-}env_{reg,,tot,nt}$	lifetime cancer risk regional, exposure via all media, non-thr.	[-]	O
$cLRman\text{-}env_{local,inh,nt}$	lifetime cancer risk local, exposure via air, non-thr.	[-]	O
$cLRman\text{-}env_{local,inh,nt}$	lifetime cancer risk regional, exposure via air, non-thr.	[-]	O

B. Margin Of Exposure

Calculation of scenario-specific MOE

Under the assumption that man is exposed throughout his or her lifetime, the total daily intake of a substance in food, drinking water and air is compared to the oral T25 or CED (BMD05), resulting in a Risk Characterisation Ratio (RCR) called the Margin Of Exposure. This comparison is made for both the local and the regional scale. In addition, the air concentration estimated for man in the standard environment can be compared to the inhalatory T25 or CED.

Depending on the available data the following RCRs are possible:

Effects / Exposure	**Exposure**	**Available effects data**
$MOEman\text{-}env_{local,tot,i}$	$DOSElocal_{tot}$	$T25_{mammal,oral,nt}$ $CED_{mammal,oral,,nt}$
$MOEman\text{-}env_{reg,tot,i}$	$DOSEreg_{tot}$	$T25_{mammal,oral,nt}$ $CED_{mammal,oral,nt}$
$MOEman\text{-}env_{local,inh,i}$	$PEClocal_{air,ann}$	$T25_{mammal,inh,nt}$ $CED_{mammal,inh,nt}$
$MOEman\text{-}env_{reg,inh,i}$	$PECreg_{air}$	$T25_{mammal,inh,nt}$ $CED_{mammal,inh,nt}$

Input

$T25_{mammal,oral,nt}$	oral T25 for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,oral,nt}$	oral CED for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$T25_{mammal,inh,nt}$	inhalatory T25 for mammals for non-threshold effects	$[kg_c.m^{-3}]$	S/O
$CED_{mammal,inh,nt}$	inhalatory CED for mammals for non-threshold effects	$[kg_c.m^{-3}]$	S/O
$DOSElocal_{tot}$	local total daily intake for humans	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$DOSEreg_{tot}$	regional total daily intake for humans	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$PEClocal_{air,ann}$	annual average local PEC in air (total)	$[kg_c.m^{-3}]$	O
$PECreg_{air}$	regional PEC in air (total)	$[kg_c.m^{-3}]$	O
	$i \in$ {repdose,carc,fert,mattox,devtox}		

Output

$MOEman\text{-}env_{local,tot,i}$	MOE local, total exposure via all media, non-thr.	[-]	O^c
$MOEman\text{-}env_{local,inh,i}$	MOE local, exposure via air, non-thr.	[-]	O^c
$MOEman\text{-}env_{reg,tot,i}$	MOE regional, total exposure via all media, non-thr.	[-]	O^c
$MOEman\text{-}env_{reg,inh,i}$	MOE regional, exposure via air, non-thr.	[-]	O^c

Derivation of scenario-specific reference-MOE

In order to account for the various uncertainties and variabilities in the extrapolation from experimental data to the human situation and in the available data set, per scenario under consideration a reference-MOE is to be derived. All aspects that can be dealt with quantitatively (as assessment factors) are combined to form the overall assessment factor or reference-MOE (RMOE).

$$RMOEman - env_{x,y,nt} = AF_{inter} \cdot AF_{allom} \cdot AF_{exprt} \cdot AF_{dose-resp} \cdot AF_{lr} \qquad \textbf{(865)}$$

$x \in$ {local,reg}

$y \in$ {tot,inh}

Input

AF_{allom}	assessment factor for allometric scaling	[-]	S/D
AF_{inter}	assessment factor for remaining interspecies differences	[-]	S/D
AF_{exprt}	assessment factor for differences in exposure route	[-]	S/D
$AF_{dose\text{-}resp}$	assessment factor for dose-response relationship	[-]	S/D
AFlr	assessment factor for extrapolation to a low risk level	[-]	S/D

Output

$RMOEman\text{-}env_{local,tot,nt}$	reference-MOE local, total exposure via all media, non-thr.	[-]	O^c
$RMOEman\text{-}env_{local,inh,nt}$	reference-MOE local, exposure via air, non-thr.	[-]	O^c
$RMOEman\text{-}env_{reg,tot,nt}$	reference-MOE regional, total exposure via all media, non-thr.	[-]	O^c
$RMOEman\text{-}env_{reg.inh,nt}$	reference-MOE regional, exposure via air, non-thr.	[-]	O^c

Comparison of MOE with reference-MOE

The MOE is compared to the reference-MOE, resulting in a MOE/reference-MOE ratio (MRR).

Depending on the available data the following MRRs are possible:

RCR / reference-MOS	**RCR**	**Reference-MOS**
$MRRman\text{-}env_{local,tot,nt}$	$MOEman\text{-}env_{local,tot,nt}$	$RMOEman\text{-}env_{local,tot,nt}$
$MRRman\text{-}env_{reg,tot,nt}$	$MOEman\text{-}env_{reg,tot,nt}$	$RMOEman\text{-}env_{reg,tot,nt}$
$MRRman\text{-}env_{local,inh,nt}$	$MOEman\text{-}env_{local,inh,nt}$	$RMOEman\text{-}env_{local,inh,nt}$
$MRRman\text{-}env_{reg,inh,nt}$	$MOEman\text{-}env_{reg,inh,nt}$	$RMOEman\text{-}env_{reg,inh,nt}$

Input

$MOEman\text{-}env_{local,tot,,nt}$	MOE local, total exposure via all media, non-thr.	[-]	O^c
$MOEman\text{-}env_{local,inh,nt}$	MOE local, exposure via air, non-thr.	[-]	O^c
$MOEman\text{-}env_{reg,tot,nt}$	MOE regional, total exposure via all media, non-thr.	[-]	O^c
$MOEman\text{-}env_{reg,inh,nt}$	MOE regional, exposure via air, non-thr.	[-]	O^c
$RMOEman\text{-}env_{local,tot,nt}$	reference-MOE local, total exposure via all media, non-thr.	[-]	O^c
$RMOEman\text{-}env_{local,inh,nt}$	reference-MOE local, exposure via air, non-thr.	[-]	O^c
$RMOEman\text{-}env_{reg,tot,nt}$	reference-MOE regional, total exposure via all media, non-thr.	[-]	O^c
$RMOEman\text{-}env_{reg.inh,nt}$	reference-MOE regional, exposure via air, non-thr.	[-]	O^c

Output

$MRRman\text{-}env_{local,tot,nt}$	ratio MOE/RMOE local, total exposure via all media, non-thr.	[-]	O^c
$MRRman\text{-}env_{reg,tot,nt}$	ratio MOE/RMOE regional, total exposure via all media, non-thr.	[-]	O^c
$MRRman\text{-}env_{local,inh,nt}$	ratio MOE/RMOE local, exposure via air, non-thr.	[-]	O^c
$MRRman\text{-}env_{reg.inh,nt}$	ratio MOE/RMOE regional, exposure via air, non-thr.	[-]	O^c

III.7.2.2 Risk characterisation for consumers

III.7.2.2.1 Threshold substances

MOS approach: Calculation of scenario-specific MOS

The concentration of the substance in air, a medium swallowed or on the skin is compared to effect or no-effect concentrations of corresponding time scale and route of exposure. Likewise, a potential dermal uptake rate for a substance in contact with the skin and an intake rate for a substance in a medium swallowed are compared to effect or no-effect doses of corresponding time scale and route of exposure. See Section III.6.2.2 for decision rules on the choice of the effect parameter in the risk characterisation for human health. If both an N(L)OAEL for man and an N(L)OAEL for mammals are available, the former one is used in this risk characterisation.

Note: Although in theory it is possible to calculate MOSs for the endpoints irritation/corrosivity and sensitisation, in practice the available toxicological database does not allow the derivation of a threshold for these endpoints. Therefore, MOS calculations for these endpoints have not been implemented in EUSES, but EUSES allows the user to flag substances for these properties (see Section III.6.2.2).

Inhalation exposure

Depending on the time scale of the exposure scenario and available effects data the following RCRs are possible:

Effects / Exposure	**Exposure**	**Available effects data**
$MOScons_{inh,acute}$	C_{inh}	$LC50_{mammal,inh}$ $NOAEL_{man,inh,acute}$ $LOAEL_{man,inh,acute}$
$MOScons_{inh,i}$	$C_{inh,ann}$	$NOAEL_{mammal,inh,i}$ $LOAEL_{mammal,inh,i}$ $NOAEL_{man,inh,i}$ $LOAEL_{man,inh,i}$ $CED_{mammal,inh,i}$

$i \in$ {repdose,carc,fert,mattox,devtox}

Input

$LC50_{mammal,inh}$	inhalatory LC50 for mammals	$[kg_c.m^{-3}]$	S
$N(L)OAEL_{man,inh,acute}$	inhalatory N(L)OAEL for man for acute effects	$[kg_c.m^{-3}]$	S
$N(L)OAEL_{mammal,inh,i}$	inhalatory N(L)OAEL for mammals for endpoint of concern	$[kg_c.m^{-3}]$	S/O
$N(L)OAEL_{man,inh,i}$	inhalatory N(L)OAEL for man for endpoint of concern	$[kg_c.m^{-3}]$	S/O
$CED_{mammal,inh,i}$	inhalatory CED for mammals for endpoint of concern	$[kg_c.m^{-3}]$	S
C_{inh}	concentration in air of room	$[kg_c.m^{-3}]$	O
$C_{inh,ann}$	annual average inhalation exposure concentration	$[kg_c.m^{-3}]$	O
	$i \in$ {repdose,carc,fert,mattox,devtox}		

Output

$MOScons_{inh,acute}$	MOS acute, inhalatory exposure	[-]	O^c
$MOScons_{inh,i}$	MOS for endpoint of concern, inhalatory exposure	[-]	O^c
	$i \in$ {repdose,carc,fert,mattox,devtox}		

Dermal exposure

Depending on the time scale of the exposure scenario and available effects data the following RCRs are possible:

Effects / Exposure	**Exposure**	**Available effects data**
$MOScons_{der,acute}$	$U_{der,pot}$	$LD50_{mammal,der}$ $NOAEL_{man,der,acute}$ $LOAEL_{man,der,acute}$
	C_{der}	$NOEC_{man,medium,acute}$ $LOEC_{man,medium,acute}$
$MOScons_{der,i}$	$U_{der,pot}$	$NOAEL_{mammal,der,i}$ $LOAEL_{mammal,der,i}$ $NOAEL_{man,der,i}$ $LOAEL_{man,der,i}$ $CED_{mammal,der,i}$
	$C_{der,ann}$	$NOEC_{man,medium,i}$ $LOEC_{man,medium,i}$

$i \in$ {repdose,carc,fert,mattox,devtox}

Input

$LD50_{mammal,der}$	dermal LD50 for mammals	$[kg_c.kg_{bw}^{-1}]$	S
$N(L)OAEL_{man,der,acute}$	dermal N(L)OAEL for man for acute effects	$[kg_c.kg_{bw}^{-1}]$	S
$N(L)OEC_{man,medium,acute}$	dermal N(L)OEC in a medium for man for acute effects	$[kg_c.m^{-3}]$	S
$N(L)OAEL_{mammal,der,i}$	dermal N(L)OAEL for mammals for endpoint of concern	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$N(L)OAEL_{man,der,i}$	dermal N(L)OAEL for man for endpoint of concern	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,der,i}$	dermal CED for mammals for endpoint of concern	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S
$N(L)OEC_{man,medium,i}$	dermal N(L)OEC in a medium for man for endpoint of concern	$[kg_c.m^{-3}]$	S
$U_{der,pot}$	potential dermal uptake rate	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
C_{der}	concentration of substance in product on skin	$[kg_c.m^{-3}]$	O
$C_{der,ann}$	annual average dermal exposure concentration	$[kg_c.m^{-3}]$	O
	$i \in$ {repdose,carc,fert,mattox,devtox}		

Output

$MOScons_{der,acute}$	MOS acute, dermal exposure	[-]	O^c
$MOScons_{der,i}$	MOS for endpoint of concern, dermal exposure	[-]	O^c
	$i \in$ {repdose,carc,fert,mattox,devtox}		

Oral exposure

Depending on the time scale of the exposure scenario and available effects data the following RCRs are possible:

Effects / Exposure	**Exposure**	**Available effects data**
$MOScons_{oral,acute}$	I_{oral}	$LD50_{mammal,oral}$ $DD_{mammal,oral}$ $NOAEL_{man,oral,acute}$ $LOAEL_{man,oral,acute}$
$MOScons_{oral,i}$	I_{oral}	$NOAEL_{mammal,oral,i}$ $LOAEL_{mammal,oral,i}$ $NOAEL_{man,oral,i}$ $LOAEL_{man,oral,i}$ $CED_{mammal,oral,i}$
	$C_{oral,ann}$ / RHO_{prod}	$NOEC_{mammal,food,i}$ $LOEC_{mammal,food,i}$

$i \in$ {repdose,carc,fert,mattox,devtox}

Input

$LD50_{mammal,oral}$	oral LD50 for mammals	$[kg_c.kg_{bw}^{-1}]$	S
$DD_{mammal,oral}$	oral Discriminating Dose for mammals	$[kg_c.kg_{bw}^{-1}]$	S
$N(L)OAEL_{man,oral,acute}$	oral N(L)OAEL for man for acute effects	$[kg_c.kg_{bw}^{-1}]$	S
$N(L)OAEL_{mammal,oral,i}$	oral N(L)OAEL for mammals for endpoint of concern	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$N(L)OAEL_{man,oral,i}$	oral N(L)OAEL for man for endpoint of concern	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,oral,i}$	oral CED for mammals for endpoint of concern	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S
$N(L)OEC_{mammal,food,i}$	N(L)OEC via food for mammals for endpoint of concern	$[kg_c.kg_{food}^{-1}]$	S
RHO_{prod}	density of product before dilution	$[kg.m^{-3}]$	S
I_{oral}	ingestion rate of substance	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$C_{oral,ann}$	annual average oral exposure concentration	$[kg_c.m^{-3}]$	O
	$i \in$ {repdose,carc,fert,mattox,devtox}		

Output

$MOScons_{oral,acute}$	MOS acute, oral exposure	[-]	O^c
$MOScons_{oral,i}$	MOS for endpoint of concern, oral exposure	[-]	O^c
	$i \in$ {repdose,carc,fert,mattox,devtox}		

Total exposure via all routes

Depending on the time scale and available effects data the following RCRs are possible:

Effects / Exposure	**Exposure**	**Available effects data**
$MOScons_{tot,acute}$	U_{tot} / $BIO_{oral,2}$	$LD50_{mammal,oral}$ $DD_{mammal,oral}$ $NOAEL_{man,oral,acute}$ $LOAEL_{man,oral,acute}$
$MOScons_{tot,i}$	U_{tot} / $BIO_{oral,2}$	$NOAEL_{mammal,oral,i}$ $LOAEL_{mammal,oral,i}$ $NOAEL_{man,oral,i}$ $LOAEL_{man,oral,i}$ $CED_{mammal,oral,i}$

$i \in$ {repdose,carc,fert,mattox,devtox}

Input

$LD50_{mammal,oral}$	oral LD50 for mammals	$[kg_c.kg_{bw}^{-1}]$	S
$DD_{mammal,oral}$	oral Discriminating Dose for mammals	$[kg_c.kg_{bw}^{-1}]$	S
$N(L)OAEL_{man,oral,acute}$	oral N(L)OAEL for man for acute effects	$[kg_c.kg_{bw}^{-1}]$	S
$N(L)OAEL_{mammal,oral,i}$	oral N(L)OAEL for mammals for endpoint of concern	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$N(L)OAEL_{man,oral,i}$	oral N(L)OAEL for man for endpoint of concern	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,oral,i}$	oral CED for mammals for endpoint of concern	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S
$BIO_{oral,2}$	bioavailability for oral uptake (starting route)	[-]	S/D
U_{tot}	total uptake for one product via different routes $i \in$ {repdose,carc,fert,mattox,devtox}	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O

Output

$MOScons_{tot,acute}$	MOS acute, total exposure	[-]	O^c
$MOScons_{tot,i}$	MOS for endpoint of concern, total exposure $i \in$ {repdose,carc,fert,mattox,devtox}	[-]	O^c

Derivation of scenario-specific reference-MOS

In order to account for the various uncertainties and variabilities in the extrapolation from experimental data to the human situation and in the available data set, per scenario under consideration a reference-MOS is to be derived. All aspects that can be dealt with quantitatively (as assessment factors) are combined to form the overall assessment factor or reference-MOS (RMOS).

$$\boldsymbol{RMOScons_{y,acute} = AF_{inter} \cdot AF_{allom} \cdot AF_{intra} \cdot AF_{expdur} \cdot AF_{exprt} \cdot AF_{dose-resp}} \qquad \textbf{(866)}$$

$$\boldsymbol{RMOScons_{y,i} = AF_{inter} \cdot AF_{allom} \cdot AF_{intra} \cdot AF_{expdur} \cdot AF_{exprt} \cdot AF_{dose-resp}} \qquad \textbf{(867)}$$

$y \in$ {inh,der,oral,tot}

$i \in$ {repdose,carc,fert,mattox,devtox}

Input

AF_{allom}	assessment factor for allometric scaling	[-]	S/D
AF_{inter}	assessment factor for remaining interspecies differences	[-]	S/D
AF_{intra}	assessment factor for intraspecies differences	[-]	S/D
AF_{expdur}	assessment factor for differences in exposure duration	[-]	S/D
AF_{exprt}	assessment factor for differences in exposure route	[-]	S/D
$AF_{dose-resp}$	assessment factor for dose-response relationship	[-]	S/D
AF_{nature}	assessment factor for nature of effect	[-]	S/D
AF_{data}	assessment factor for adequacy of/confidence in database	[-]	S/D

Output

$RMOScons_{inh,acute}$	reference-MOS inhalatory exposure, for acute toxicity	[-]	O^c
$RMOScons_{der,acute}$	reference-MOS dermal exposure, for acute toxicity	[-]	O^c
$RMOScons_{oral,acute}$	reference-MOS oral exposure, for acute toxicity	[-]	O^c
$RMOScons_{tot,acute}$	reference-MOS total exposure, for acute toxicity	[-]	O^c
$RMOScons_{inh,i}$	reference-MOS inhalatory exposure, for endpoint of concern	[-]	O^c
$RMOScons_{der,i}$	reference-MOS dermal exposure, for endpoint of concern	[-]	O^c
$RMOScons_{oral,i}$	reference-MOS oral exposure, for endpoint of concern	[-]	O^c
$RMOScons_{tot,i}$	reference-MOS total exposure, for endpoint of concern	[-]	O^c

$i \in \{repdose,carc,fert,mattox,devtox\}$

Comparison of MOS with reference-MOS

In judging the acceptability of the MOS, in a second step of the quantitative risk characterisation the MOS is compared to the reference-MOS, resulting in a MOS/reference-MOS ratio (MRR).

Depending on the available data the following MRRs are possible:

RCR / reference-MOS	**RCR**	**reference-MOS**
$MRRcons_{inh,acute}$	$MOScons_{inh,acute}$	$RMOScons_{inh,acute}$
$MRRcons_{inh,i}$	$MOScons_{inh,i}$	$RMOScons_{inh,i}$
$MRRcons_{der,acute}$	$MOScons_{der,acute}$	$RMOScons_{der,acute}$
$MRRcons_{der,i}$	$MOScons_{der,i}$	$RMOScons_{der,i}$
$MRRcons_{oral,acute}$	$MOScons_{oral,acute}$	$RMOScons_{oral,acute}$
$MRRcons_{oral,i}$	$MOScons_{oral,i}$	$RMOScons_{oral,i}$
$MRRcons_{tot,acute}$	$MOScons_{tot,acute}$	$RMOScons_{tot,acute}$
$MRRcons_{tot,i}$	$MOScons_{tot,i}$	$RMOScons_{tot,i}$

$i \in \{repdose,carc,fert,mattox,devtox\}$

Input

$MOScons_{inh,acute}$	MOS acute, inhalatory exposure	[-]	O^c
$MOScons_{inh,i}$	MOS for endpoint of concern, inhalatory exposure	[-]	O^c
$MOScons_{der,acute}$	MOS acute, dermal exposure	[-]	O^c
$MOScons_{der,i}$	MOS for endpoint of concern, dermal exposure	[-]	O^c
$MOScons_{oral,acute}$	MOS acute, oral exposure	[-]	O^c
$MOScons_{oral,i}$	MOS for endpoint of concern, oral exposure	[-]	O^c
$MOScons_{tot,acute}$	MOS acute, total exposure	[-]	O^c
$MOScons_{tot,i}$	MOS for endpoint of concern, total exposure	[-]	O^c
$RMOScons_{inh,acute}$	reference-MOS inhalatory exposure, for acute toxicity	[-]	O^c
$RMOScons_{der,acute}$	reference-MOS dermal exposure, for acute toxicity	[-]	O^c
$RMOScons_{oral,acute}$	reference-MOS oral exposure, for acute toxicity	[-]	O^c
$RMOScons_{tot,acute}$	reference-MOS total exposure, for acute toxicity	[-]	O^c
$RMOScons_{inh,i}$	reference-MOS inhalatory exposure, for endpoint of concern	[-]	O^c
$RMOScons_{der,i}$	reference-MOS dermal exposure, for endpoint of concern	[-]	O^c
$RMOScons_{oral,i}$	reference-MOS oral exposure, for endpoint of concern	[-]	O^c
$RMOScons_{tot,i}$	reference-MOS total exposure, for endpoint of concern	[-]	O^c
	$i \in$ {repdose,carc,fert,mattox,devtox}		

Output

$MRRcons_{inh,acute}$	ratio MOS/reference-MOS inhalatory exposure, for acute toxicity	[-]	O^c
$MRRcons_{der,acute}$	ratio MOS/reference-MOS dermal exposure, for acute toxicity	[-]	O^c
$MRRcons_{oral,acute}$	ratio MOS/reference-MOS oral exposure, for acute toxicity	[-]	O^c
$MRRcons_{tot,acute}$	ratio MOS/reference-MOS total exposure, for acute toxicity	[-]	O^c
MRRconsinh,i	ratio MOS/reference-MOS inhalatory exposure, for endpoint of concern	[-]	Oc
MRRconsder,i	ratio MOS/reference-MOS dermal exposure, for endpoint of concern	[-]	Oc
MRRconsoral,i	ratio MOS/reference-MOS oral exposure, for endpoint of concern	[-]	Oc
MRRconstot,i	ratio MOS/reference-MOS total exposure, for endpoint of concern	[-]	Oc
	$i \in$ {repdose,carc,fert,mattox,devtox}		

III.7.2.2.2 Method for non-threshold based effects

A. Lifetime carcinogenic risk

Starting point is the T25 which first needs to be converted to an equivalent human dose descriptor, the HT25, applying allometric assessment factors and, possibly, an assessment factor for route-to-route extrapolation.

$$\boldsymbol{AFcons_{x,nt} = AF_{allom} \cdot AF_{\exp rt}} \tag{868}$$

$x \in$ {inh,der,oral,tot}

Input

AF_{allom}	assessment factor for allometric scaling	[-]	S/D
AF_{exprt}	assessment factor for differences in exposure route	[-]	S/D

Output

$AFcons_{linh,nt}$	assessment factor for inhalatory exposure, non-thr.	[-]	S/O
$AFcons_{der,nt}$	assessment factor for dermal exposure, non-thr.	[-]	S/O
$AFcons_{oral,nt}$	assessment factor for oral exposure, non-thr.	[-]	S/O
$AFcons_{tot,nt}$	assessment factor for total exposure, non-thr.	[-]	S/O

$$\boldsymbol{HT25cons_{x,nt} = \frac{T25_{mammal,x,nt}}{AFcons_{x,nt}}} \tag{869}$$

$x \in$ {inh, der,oral,tot}

Input

$T25_{mammal,inh,nt}$	inhalatory T25 for mammals for non-threshold effects	$[kg_c.m^{-3}]$	S/O
$T25_{mammal,der,nt}$	dermal T25 for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$T25_{mammal,oral,nt}$	oral T25 for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$AFcons_{linh,nt}$	assessment factor for inhalatory consumer exposure, non-thr.	[-]	S/O
$AFcons_{der,nt}$	assessment factor for dermal consumer exposure, non-thr.	[-]	S/O
$AFcons_{oral,nt}$	assessment factor for oral consumer exposure, non-thr.	[-]	S/O
$AFcons_{tot,nt}$	assessment factor for total consumer exposure, non-thr.	[-]	S/O

Output

$HT25cons_{inh,nt}$	human equivalent dose inhalatory consumer exposure, non-thr.	$[kg_c.m^{-3}]$	O
$HT25cons_{der,nt}$	human equivalent dose dermal consumer exposure, non-thr.	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$HT25cons_{oral,nt}$	human equivalent dose oral consumer exposure, non-thr.	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$HT25cons_{tot,nt}$	human equivalent dose total consumer exposure, non-thr.	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O

Subsequently the lifetime cancer risk is calculated for each route of exposure.

$$cLRcons_{inh,nt} = \frac{C_{inh,ann}}{HT25cons_{inh,nt}} \cdot 0.25 \tag{870}$$

$$cLRcons_{der,nt} = \frac{U_{der,pot}}{HT25cons_{der,nt}} \cdot 0.25 \tag{871}$$

$$cLRcons_{oral,nt} = \frac{I_{oral}}{HT25cons_{oral,nt}} \cdot 0.25 \tag{872}$$

$$cLRcons_{tot,nt} = \frac{U_{tot}}{HT25cons_{tot,nt}} \cdot 0.25 \tag{873}$$

Input

C_{inh}	annual average inhalation exposure concentration	$[kg_c.m^{-3}]$	O
$U_{der,pot}$	potential dermal uptake rate	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
I_{oral}	ingestion rate of substance	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
U_{tot}	total uptake for one product via different routes	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$HT25cons_{inh,nt}$	human equivalent dose inhalatory consumer exposure, non-thr.	$[kg_c.m^{-3}]$	O
$HT25cons_{der,nt}$	human equivalent dose dermal consumer exposure, non-thr.	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$HT25cons_{oral,nt}$	human equivalent dose oral consumer exposure, non-thr.	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$HT25cons_{tot,nt}$	human equivalent dose total consumer exposure, non-thr.	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O

Output

$cLRcons_{inh,nt}$	lifetime cancer risk, inhalatory consumer exposure, non-thr.	[-]	O
$cLRcons_{der,nt}$	lifetime cancer risk, dermal consumer exposure, non-thr.	[-]	O
$cLRcons_{oral,nt}$	lifetime cancer risk oral consumer exposure, non-thr.	[-]	O
$cLRcons_{tot,nt}$	lifetime cancer risk, total consumer exposure, non-thr.	[-]	O

B. Margin Of Exposure

Calculation of scenario-specific MOE

Under the assumption that man is exposed throughout his or her lifetime, consumer exposure to a substance is compared to the T25 or CED (BMD05), resulting in a Risk Characterisation Ratio (RCR) called the Margin Of Exposure. This comparison is made for all routes of exposure.

Depending on the available data the following RCRs are possible:

Effects / Exposure	**Exposure**	**Available effects data**
$MOEcons_{inh,nt}$	$C_{inh,ann}$	$T25_{mammal,inh,nt}$ $CED_{mammal,inh,,nt}$
$MOEcons_{der,nt}$	$U_{der,pot}$	$T25_{mammal,der,nt}$ $CED_{mammal,der,nt}$
$MOEcons_{oral,nt}$	I_{oral}	$T25_{mammal,oral,nt}$ $CED_{mammal,oral,nt}$
$MOEcons_{tot,nt}$	$U_{tot}/BIO_{oral,2}$	$T25_{mammal,oral,nt}$ $CED_{mammal,oral,nt}$

Input

$T25_{mammal,inh,nt}$	inhalatory T25 for mammals for non-threshold effects	$[kg_c.m^{-3}]$	S/O
$CED_{mammal,inh,nt}$	inhalatory CED for mammals for non-threshold effects	$[kg_c.m^{-3}]$	S/O
$T25_{mammal,der,nt}$	dermal T25 for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,der,nt}$	dermal CED for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$T25_{mammal,oral,nt}$	oral T25 for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,oral,nt}$	oral CED for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
C_{inh}	annual average inhalation exposure concentration	$[kg_c.m^{-3}]$	O
$U_{der,pot}$	potential dermal uptake rate	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
I_{oral}	ingestion rate of substance	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
U_{tot}	total uptake for one product via different routes	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$BIO_{oral,2}$	bioavailability for oral uptake, starting route		

Output

$MOEcons_{inh,nt}$	MOE inhalatory consumer exposure, non-thr.	[-]	O^c
$MOEcons_{der,nt}$	MOE dermal consumer exposure, non-thr.	[-]	O^c
$MOEcons_{oral,nt}$	MOE oral consumer exposure, non-thr.	[-]	O^c
$MOEcons_{tot,nt}$	MOE total consumer exposure, non-thr.	[-]	O^c

Derivation of scenario-specific reference-MOE

In order to account for the various uncertainties and variabilities in the extrapolation from experimental data to the consumer situation and in the available data set, per scenario under consideration a reference-MOE is to be derived. All aspects that can be dealt with quantitatively (as assessment factors) are combined to form the overall assessment factor or reference-MOE (RMOE).

$$\boldsymbol{RMOEcons_{x,nt} = AF_{inter} \cdot AF_{allom} \cdot AF_{exprt} \cdot AF_{dose-resp} \cdot AF_{lr}} \qquad \textbf{(874)}$$

$x \in \{inh,der,oral,tot\}$

Input

AF_{allom}	assessment factor for allometric scaling	[-]	S/D
AF_{inter}	assessment factor for remaining interspecies differences	[-]	S/D
AF_{exprt}	assessment factor for differences in exposure route	[-]	S/D
$AF_{dose\text{-}resp}$	assessment factor for dose-response relationship	[-]	S/D
AFlr	assessment factor for extrapolation to a low risk level	[-]	S/D

Output

$RMOEcons_{inh,nt}$	reference-MOE inhalatory consumer exposure, non-thr.	[-]	O^c
$RMOEcons_{der,nt}$	reference-MOE dermal consumer exposure, non-thr.	[-]	O^c
$RMOEcons_{oral,nt}$	reference-MOE oral consumer exposure, non-thr.	[-]	O^c
$RMOEcons_{tot,nt}$	reference-MOE total consumer exposure, non-thr.	[-]	O^c

Comparison of MOE with reference-MOE

The MOE is compared to the reference-MOE, resulting in a MOE/reference-MOE ratio (MRR).

Depending on the available data the following MRRs are possible:

RCR / reference-MOS	**RCR**	**Reference-MOS**
$MRRcons_{inh,nt}$	$MOEcons_{inh,nt}$	$RMOEcons_{inh,nt}$
$MRRcons_{der,nt}$	$MOEcons_{der,nt}$	$RMOEcons_{der,nt}$
$MRRcons_{oral,nt}$	$MOEcons_{oral,nt}$	$RMOEcons_{oral,nt}$
$MRRcons_{tot,nt}$	$MOEcons_{tot,nt}$	$RMOEcons_{tot,nt}$

Input

$MOEcons_{inh,nt}$	MOE inhalatory consumer exposure, non-thr.	[-]	O^c
$MOEcons_{der,nt}$	MOE dermal consumer exposure, non-thr.	[-]	O^c
$MOEcons_{oral,nt}$	MOE oral consumer exposure, non-thr.	[-]	O^c
$MOEcons_{tot,nt}$	MOE total consumer exposure, non-thr.	[-]	O^c
$RMOEcons_{inh,nt}$	reference-MOE inhalatory consumer exposure, non-thr.	[-]	O^c
$RMOEcons_{der,nt}$	reference-MOE dermal consumer exposure, non-thr.	[-]	O^c
$RMOEcons_{oral,nt}$	reference-MOE oral consumer exposure, non-thr.	[-]	O^c
$RMOEcons_{tot,nt}$	reference-MOE total consumer exposure, non-thr.	[-]	O^c

Output

$MRRcons_{inh,nt}$	ratio MOE/RMOE, inhalatory consumer exposure, non-thr.	[-]	O^c
$MRRcons_{der,nt}$	ratio MOE/RMOE, dermal consumer exposure, non-thr.	[-]	O^c
$MRRcons_{oral,nt}$	ratio MOE/RMOE, oral consumer exposure, non-thr.	[-]	O^c
$MRRcons_{tot,nt}$	ratio MOE/RMOE, total consumer exposure, non-thr.	[-]	O^c

III.7.2.3 Risk characterisation for workers

III.7.2.3.1 Threshold substances

MOS approach: Calculation of scenario-specific MOS

For the (sub-)chronic endpoints, the output of the EASE model is compared to effect or no-effect concentrations of corresponding route of exposure. For the acute endpoints, MOS calculations are based on acute exposure data which have been introduced in EUSES separately. See Section III.6.2.2 for decision rules on the choice of the effect parameter in the risk characterisation for human health. If both an N(L)OAEL for man and an N(L)OAEL for mammals are available, the former one is used in this risk characterisation.

Note: Although in theory it is possible to calculate MOSs for the endpoints irritation/corrosivity and sensitisation, in practice the available toxicological database does not allow the derivation of a threshold for these endpoints. Therefore, MOS calculations for these endpoints have not been implemented in EUSES, but EUSES allows the user to flag substances for these properties.

Inhalation exposure

Depending on the time scale of the exposure scenario and available effects data the following RCRs are possible:

Effects / Exposure	**Exposure**	**Available effects data**
$MOSworker_{inh,acute}$	$C_{inh,worker,acute}$	$LC50_{mammal,inh}$ $NOAEL_{man,inh,acute}$ $LOAEL_{man,inh,acute}$
$MOSworker_{inh,vapour,i}$	$C_{inh,worker,vapour}$	$NOAEL_{mammal,inh,i}$ $LOAEL_{mammal,inh,i}$ $NOAEL_{man,inh,i}$ $LOAEL_{man,inh,i}$ $CED_{mammal,inh,i}$
$MOSworker_{inh,fibre,i}$	$C_{inh,worker,fibre}$	$NOAEL_{mammal,inh,fibre,i}$ $LOAEL_{mammal,inh,fibre,i}$ $NOAEL_{man,inh,fibre,i}$ $LOAEL_{man,inh,fibre,i}$ $CED_{mammal,inh,fibre,i}$
$MOSworker_{inh,dust,i}$	$C_{inh,worker,dust}$	$NOAEL_{mammal,inh,i}$ $LOAEL_{mammal,inh,i}$ $NOAEL_{man,inh,i}$ $LOAEL_{man,inh,i}$ $CED_{mammal,inh,i}$

$i \in \{repdose,carc,fert,mattox,devtox\}$

Input

$LC50_{mammal,inh}$	inhalatory LC50 for mammals	[kg$_c$.m^{-3}]	S
$N(L)OAEL_{man,inh,acute}$	inhalatory N(L)OAEL for man for acute effects	[kg$_c$.m^{-3}]	S
$N(L)OAEL_{mammal,inh,i}$	inhalatory N(L)OAEL for mammals for endpoint of concern	[kg$_c$.m^{-3}]	S/O
$N(L)OAEL_{man,inh,i}$	inhalatory N(L)OAEL for man for endpoint of concern	[kg$_c$.m^{-3}]	S/O
$CED_{mammal,inh,i}$	inhalatory CED for mammals for endpoint of concern	[kg$_c$.m^{-3}]	S
$N(L)OAEL_{mammal,inh,fibre,i}$	inh. N(L)OAEL for mammals exposed to fibers for endpoint of concern	[fibers.m^{-3}]	S
$N(L)OAEL_{man,inh,fibre,i}$	inh. N(L)OAEL for man exposed to fibers for endpoint of concern	[fibers.m^{-3}]	S
$CED_{mammal,inh,fibre,i}$	inh. CED for mammals exposed to fibers for endpoint of concern	[fibers.m^{-3}]	S
$C_{inh,worker,acute}$	concentration in air for workers, acute exposure	[kg.m^{-3}]	S
$C_{inh,worker,vapour}$	vapour concentration in air for workers	[kg.m^{-3}]	O
$C_{inh,worker,fibre}$	fibre concentration in air for workers	[fibers.m^{-3}]	O
$C_{inh,worker,dust}$	dust concentration in air for workers	[kg.m^{-3}]	O
	i ∈ {repdose,carc,fert,mattox,devtox}		

Output

$MOSworker_{inh,acute}$	MOS acute, inhalatory exposure	[-]	O^c
$MOSworker_{inh,vapour,i}$	MOS for endpoint of concern, inhalatory exposure of vapour	[-]	O^c
$MOSworker_{inh,fibre,i}$	MOS for endpoint of concern, inhalatory exposure of fibers	[-]	O^c
$MOSworker_{inh,dust,i}$	MOS for endpoint of concern, inhalatory exposure of dust	[-]	O^c
	i ∈ {repdose,carc,fert,mattox,devtox}		

Dermal exposure

Depending on the time scale of the exposure scenario and available effects data the following RCRs are possible:

Effects / Exposure	**Exposure**	**Available effects data**
$MOSworker_{der,acute}$	$U_{der,pot,worker,acute}$	$LD50_{mammal,der}$ $NOAEL_{man,der,acute}$ $LOAEL_{man,der,acute}$
	$W_{der,worker,acute} / (TH_{der,worker} \cdot n_{worker})$	$NOEC_{man,medium,acute}$ $LOEC_{man,medium,acute}$
$MOSworker_{der,i}$	$U_{der,pot,worker}$	$NOAEL_{mammal,der,i}$ $LOAEL_{mammal,der,i}$ $NOAEL_{man,der,i}$ $LOAEL_{man,der,i}$ $CED_{mammal,der,i}$
	$W_{der,worker} / (TH_{der,worker} \cdot n_{worker})$	$NOEC_{man,medium,i}$ $LOEC_{man,medium,i}$

i ∈ {repdose,carc,fert,mattox,devtox}

Input

$LD50_{mammal,der}$	dermal LD50 for mammals	$[kg_c.kg_{bw}^{-1}]$	S
$N(L)OAEL_{man,der,acute}$	dermal N(L)OAEL for man for acute effects	$[kg_c.kg_{bw}^{-1}]$	S
$N(L)OEC_{man,medium,acute}$	dermal N(L)OEC in a medium for man for acute effects	$[kg_c.m^{-3}]$	S
$N(L)OAEL_{mammal,der,i}$	dermal N(L)OAEL for mammals for endpoint of concern	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$N(L)OAEL_{man,der,i}$	dermal N(L)OAEL for man for endpoint of concern	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,der,i}$	dermal CED for mammals for endpoint of concern	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S
$N(L)OEC_{man,medium,i}$	dermal N(L)OEC in a medium for man for endpoint of concern	$[kg_c.m^{-3}]$	S
$U_{der,pot,worker,acute}$	potential dermal uptake for workers, acute exposure	$[kg.kg_{bw}^{-1}.d^{-1}]$	S
$W_{der,worker,acute}$	dermal weight of substance on skin of worker per day, acute exp.	$[kg.m^{-2}.d^{-1}]$	S
$U_{der,pot,worker}$	potential dermal uptake for workers	$[kg.kg_{bw}^{-1}.d^{-1}]$	O
$W_{der,worker}$	dermal weight of substance on skin of worker per day	$[kg.m^{-2}.d^{-1}]$	O
$TH_{der,worker}$	thickness of product	[m]	D
n_{worker}	mean number of events per day	$[d^{-1}]$	S
	i ∈ {repdose,carc,fert,mattox,devtox}		

Output

$MOSworker_{der,acute}$	MOS acute, dermal exposure	[-]	O^c
$MOSworker_{der,i}$	MOS for endpoint of concern, dermal exposure	[-]	O^c
	i ∈ {repdose,carc,fert,mattox,devtox}		

Total exposure

For certain scenarios there may be both dermal and inhalation exposure. Depending on the time scale of the exposure scenario and available effects data the following RCRs are possible:

Effects / Exposure	**Exposure**	**Available effects data**
$MOSworker_{tot,acute}$	$U_{tot,worker,acute}$ / $BIO_{oral,2}$	$LD50_{mammal,oral}$ $DD_{mammal,oral}$ $NOAEL_{man,oral,acute}$ $LOAEL_{man,oral,acute}$
$MOSworker_{tot-v/d,i}$	$U_{tot-v/d,worker}$ / $BIO_{oral,2}$	$NOAEL_{mammal,oral,i}$ $LOAEL_{mammal,oral,i}$ $NOAEL_{man,oral,i}$ $LOAEL_{man,oral,i}$ $CED_{mammal,oral,i}$

i ∈ {repdose,carc,fert,mattox,devtox}

Input

$LD50_{mammal,oral}$	oral LD50 for mammals	$[kg_c.kg_{bw}^{-1}]$	S
$DD_{mammal,oral}$	oral Discriminating Dose for mammals	$[kg_c.kg_{bw}^{-1}]$	S
$N(L)OAEL_{man,oral,acute}$	oral N(L)OAEL for man for acute effects	$[kg_c.kg_{bw}^{-1}]$	S
$N(L)OAEL_{mammal,oral,i}$	oral N(L)OAEL for mammals for endpoint of concern	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$N(L)OAEL_{man,oral,i}$	oral N(L)OAEL for man for endpoint of concern	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,oral,i}$	oral CED for mammals for endpoint of concern	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S
$BIO_{oral,2}$	bioavailability for oral uptake (starting route)	[-]	S/D
$U_{tot,worker,acute}$	total uptake for one scenario via different routes, for acute effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$U_{tot\text{-}v/d,worker}$	total uptake (vapour + dermal) for one scenario via diff. routes	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
	$i \in$ {repdose,carc,fert,mattox,devtox}		

Output

$MOSworker_{tot,acute}$	MOS acute, total exposure	[-]	O^c
$MOSworker_{tot\text{-}v/d,i}$	MOS for endpoint of concern, total exposure (vapour + dermal)	[-]	O^c
	$i \in$ {repdose,carc,fert,mattox,devtox}		

Derivation of scenario-specific reference-MOS

In order to account for the various uncertainties and variabilities in the extrapolation from experimental data to the human situation and in the available data set, per scenario under consideration a reference-MOS is to be derived. All aspects that can be dealt with quantitatively (as assessment factors) are combined to form the overall assessment factor or reference-MOS (RMOS).

$$RMOSworker_{y,acute} = AF_{inter} \cdot AF_{allom} \cdot AF_{intra} \cdot AF_{expdur} \cdot AF_{exprt} \cdot AF_{dose-resp} \tag{875}$$

$$RMOSworker_{z,i} = AF_{inter} \cdot AF_{allom} \cdot AF_{intra} \cdot AF_{expdur} \cdot AF_{exprt} \cdot AF_{dose-resp} \cdot CF_{occup1} \tag{876}$$

$y \in$ {inh,der,tot}
$z \in$ {inh-vapour,inh-fibre,inh-dust,der,tot-v/d}
$i \in$ {repdose,carc,fert,mattox,devtox}

Input

AF_{allom}	assessment factor for allometric scaling	[-]	S/D
AF_{inter}	assessment factor for remaining interspecies differences	[-]	S/D
AF_{intra}	assessment factor for intraspecies differences	[-]	S/D
AF_{expdur}	assessment factor for differences in exposure duration	[-]	S/D
AF_{exprt}	assessment factor for differences in exposure route	[-]	S/D
$AF_{dose-resp}$	assessment factor for dose-response relationship	[-]	S/D
AF_{nature}	assessment factor for nature of effect	[-]	S/D
AF_{data}	assessment factor for adequacy of/confidence in database	[-]	S/D
CF_{occup1}	correction factor for respiratory rate in route-to-route extrapolation	[-]	S/D

Output

$RMOSworker_{inh,acute}$	reference-MOS inhalatory exposure, for acute toxicity	[-]	O^c
$RMOSworker_{der,acute}$	reference-MOS dermal exposure, for acute toxicity	[-]	O^c
$RMOSworker_{tot,acute}$	reference-MOS total exposure, for acute toxicity	[-]	O^c
$RMOSworker_{inh\text{-}vapour,i}$	reference-MOS inhalatory exposure of vapour, for endpoint of concern	[-]	O^c
$RMOSworker_{inh\text{-}fibre,i}$	reference-MOS inhalatory exposure of fibers, for endpoint of concern	[-]	O^c
$RMOSworker_{inh\text{-}dust,i}$	reference-MOS inhalatory exposure of dust, for endpoint of concern	[-]	O^c
$RMOSworker_{der,i}$	reference-MOS dermal exposure, for endpoint of concern	[-]	O^c
$RMOSworker_{tot\text{-}v/d,i}$	reference-MOS total exposure (vapour + dermal), for endpoint of concern	[-]	O^c
	$i \in$ {repdose,carc,fert,mattox,devtox}		

For the route-to-route extrapolation for workers involving the inhalatory route an additional correction is used to account for the difference between the respiratory rate of the general population (default 20 m3 per 24 hrs) used in the route-to-route extrapolation and the respiratory rate of workers (10 m3 in 8 hrs). The TGD recommends a factor of 0.5 for extrapolations from the dermal and oral route to the inhalatory route and 2 for extrapolations from the inhalatory route to the dermal and oral route. EUSES allows this correction in the derivation of the RMOS, RMOE and human equivalent dose for workers. The default is 1.

Comparison of MOS with reference-MOS

In judging the acceptability of the MOS, in a second step of the quantitative risk characterisation the MOS is compared to the reference-MOS, resulting in a MOS/reference-MOS ratio (MRR).

Depending on the available data the following MRRs are possible:

RCR / reference-MOS	**RCR**	**reference-MOS**
$MRRworker_{inh,acute}$	$MOSworker_{inh,acute}$	$RMOSworker_{inh,acute}$
$MRRworker_{inh-vapour,i}$	$MOSworker_{inh-vapour,i}$	$RMOSworker_{inh-vapour,i}$
$MRRworker_{inh-fibre,i}$	$MOSworker_{inh-fibre,i}$	$RMOSworker_{inh-fibre,i}$
$MRRworker_{inh-dust,i}$	$MOSworker_{inh-dust,i}$	$RMOSworker_{inh-dust,i}$
$MRRworker_{der,acute}$	$MOSworker_{der,acute}$	$RMOSworker_{der,acute}$
$MRRworker_{der,i}$	$MOSworker_{der,i}$	$RMOSworker_{der,i}$
$MRRworker_{tot,acute}$	$MOSworker_{tot,acute}$	$RMOSworker_{tot,acute}$
$MRRworker_{tot-v/d,i}$	$MOSworker_{tot-v/d,i}$	$RMOSworker_{tot-v/d,i}$

$i \in$ {repdose,carc,fert,mattox,devtox}

Input

$MOSworker_{inh,acute}$	MOS acute, inhalatory exposure	[-]	O^c
$MOSworker_{inh,vapour,i}$	MOS for endpoint of concern, inhalatory exposure of vapour	[-]	O^c
$MOSworker_{inh,fibre,i}$	MOS for endpoint of concern, inhalatory exposure of fibers	[-]	O^c
$MOSworker_{inh,dust,i}$	MOS for endpoint of concern, inhalatory exposure of dust	[-]	O^c
$MOSworker_{der,acute}$	MOS acute, dermal exposure	[-]	O^c
$MOSworker_{der,i}$	MOS for endpoint of concern, dermal exposure	[-]	O^c
$MOSworker_{tot,acute}$	MOS acute, total exposure	[-]	O^c
$MOSworker_{tot\text{-}v/d,i}$	MOS for endpoint of concern, total exposure (vapour + dermal)	[-]	O^c
$RMOSworker_{inh,acute}$	reference-MOS inhalatory exposure, for acute toxicity	[-]	O^c
$RMOSworker_{der,acute}$	reference-MOS dermal exposure, for acute toxicity	[-]	O^c
$RMOSworker_{tot,acute}$	reference-MOS total exposure, for acute toxicity	[-]	O^c
$RMOSworker_{inh\text{-}vapour,i}$	reference-MOS inhalatory exposure of vapour, for endpoint of concern	[-]	O^c
$RMOSworker_{inh\text{-}fibre,i}$	reference-MOS inhalatory exposure of fibers, for endpoint of concern	[-]	O^c
$RMOSworker_{inh\text{-}dust,i}$	reference-MOS inhalatory exposure of dust, for endpoint of concern	[-]	O^c
$RMOSworker_{der,i}$	reference-MOS dermal exposure, for endpoint of concern	[-]	O^c
$RMOSworker_{tot\text{-}v/d,i}$	reference-MOS total exposure (vapour + dermal), for endpoint of concern	[-]	O^c
	$i \in$ {repdose,carc,fert,mattox,devtox}		

Output

$MRRworker_{inh,acute}$	ratio MOS/reference-MOS inhalatory exposure, for acute toxicity	[-]	O^c
$MRRworker_{der,acute}$	ratio MOS/reference-MOS dermal exposure, for acute toxicity	[-]	O^c
$MRRworker_{tot,acute}$	ratio MOS/reference-MOS total exposure, for acute toxicity	[-]	O^c
$MRRworker_{inh\text{-}vapour,i}$	ratio MOS/reference-MOS inhalatory exposure of vapour, for endpoint of concern	[-]	O^c
$MRRworker_{inh\text{-}fibre,i}$	ratio MOS/reference-MOS inhalatory exposure of fibers, for endpoint of concern	[-]	O^c
$MRRworker_{inh\text{-}dust,i}$	ratio MOS/reference-MOS inhalatory exposure of dust, for endpoint of concern	[-]	O^c
$MRRworker_{der,i}$	ratio MOS/reference-MOS dermal exposure, for endpoint of concern	[-]	O^c
$MRRworker_{tot\text{-}v/d,i}$	ratio MOS/reference-MOS total exposure (vapour + dermal), for endpoint of concern	[-]	O^c
	$i \in$ {repdose,carc,fert,mattox,devtox}		

III.7.2.3.2 Non-threshold substances

A. Lifetime carcinogenic risk

Starting point is the T25 which first needs to be converted to an equivalent human dose descriptor, the HT25, applying allometric assessment factors and, possibly, an assessment factor for route-to-route extrapolation.

$$AFworker_{x,nt} = AF_{allom} \cdot AF_{exprt} . CF_{occup1} \qquad \textbf{(877)}$$

$x \in$ {inh-vapour,inh-fibre, inh-dust, der,tot-v/d}

Input

AF_{allom}	assessment factor for allometric scaling	[-]	S/D
AF_{exprt}	assessment factor for differences in exposure route	[-]	S/D
CF_{occup1}	correction factor for respiratory rate in route-to-route extrapolation	[-]	S/D

Output

$AFworker_{linh\text{-}vaour,nt}$	assessment factor for inhalatory worker vapour exposure, non-thr.	[-]	S/O
$AFworker_{linh\text{-}fibre,nt}$	assessment factor for inhalatory worker fibre exposure, non-thr.	[-]	S/O
$AFworker_{linh\text{-}dust,nt}$	assessment factor for inhalatory worker dust exposure, non-thr.	[-]	S/O
$AFworker_{der,nt}$	assessment factor for dermal worker exposure, non-thr.	[-]	S/O
$AFworker_{tot\text{-}v/d,nt}$	assessment factor for total worker exposure, non-thr.	[-]	S/O

$$HT25worker_{x,nt} = \frac{T25_{mammal,x,nt}}{AFworker_{x,nt}} \tag{878}$$

$x \in$ {inh-vapour,inh-fibre, inh-dust, der,tot-v/d}

Input			
$T25_{mammal,inh,,nt}$	inhalatory T25 for mammals for non-threshold effects	[$kg_c.m^{-3}$]	S/O
$T25_{mammal,inh,fibre,nt}$	inhalatory T25 (fibre)for mammals for non-threshold effects	[$fibres.m^{-3}$]	S/O
$T25_{mammal,inh,dust,nt}$	inhalatory T25 (dust) for mammals for non-threshold effects	[$kg_c.m^{-3}$]	S/O
$T25_{mammal,der,nt}$	dermal T25 for mammals for non-threshold effects	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	S/O
$AFworker_{inh-vapour,nt}$	assessment factor for inhalatory worker vapour exposure, non-thr.	[-]	S/O
$AFworker_{inh-fibre,nt}$	assessment factor for inhalatory worker fibre exposure, non-thr.	[-]	S/O
$AFworker_{inh-dust,nt}$	assessment factor for inhalatory worker dust exposure, non-thr.	[-]	S/O
$AFworker_{der,nt}$	assessment factor for dermal worker exposure, non-thr.	[-]	S/O
$AFworker_{tot-v/d,nt}$	assessment factor for total worker exposure, non-thr.	[-]	S/O
Output			
$HT25worker_{inh,vapour,nt}$	human equivalent dose inhalatory worker vapour exposure, non-thr.	[$kg_c.m^{-3}$]	O
$HT25worker_{inh,fibr,nt}$	human equivalent dose inhalatory worker fibre exposure, non-thr.	[$fibres.m^{-3}$]	O
$HT25worker_{inh,dust,nt}$	human equivalent dose inhalatory worker dust exposure, non-thr.	[$kg_c.m^{-3}$]	O
$HT25worker_{der,nt}$	human equivalent dose dermal worker exposure, non-thr.	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O
$HT25worker_{tot-v/d,nt}$	human equivalent dose total worker exposure, non-thr.	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O

For the route-to-route extrapolation for workers involving the inhalatory route an additional correction is used to account for the difference between the respiratory rate of the general population (default 20 m3 per 24 hrs) used in the route-to-route extrapolation and the respiratory rate of workers (10 m3 in 8 hrs). The TGD recommends a factor of 0.5 for extrapolations from the dermal and oral route to the inhalatory route and 2 for extrapolations from the inhalatory route to the dermal and oral route. EUSES allows this correction in the derivation of the RMOS, RMOE and human equivalent dose for workers. The default is 1.

Subsequently the lifetime cancer risk is calculated for each route of exposure. The exposure is corrected for differences between occupational and lifetime conditions by dividing by a factor of 2.8 (default = 7/5 . 52/48 . 75/40 = 2.8).

$$cLRworker_{inh,vapour,nt} = \frac{C_{inh,worker,vapour}}{HT25worker_{inh,vapour,nt}} \cdot 0.25.\frac{1}{CF_{occup2}} \tag{879}$$

$$cLRworker_{inh,fibre,nt} = \frac{C_{inh,worker,fibre}}{HT25worker_{inh,fibre,nt}} \cdot 0.25.\frac{1}{CF_{occup2}} \tag{880}$$

$$cLRworker_{inh,dust,nt} = \frac{C_{inh,worker,dust}}{HT25worker_{inh,dust,nt}} \cdot 0.25.\frac{1}{CF_{occup2}} \tag{881}$$

$$cLRworker_{der,nt} = \frac{U_{der,pot,worker}}{HT25worker_{der,nt}} \cdot 0.25.\frac{1}{CF_{occup2}} \tag{882}$$

$$cLRworker_{tot-v/d,nt} = \frac{U_{tot-v/d,worker}}{HT25worker_{tot-v/d,nt}} \cdot 0.25.\frac{1}{CF_{occup2}} \tag{883}$$

Input

$C_{inh,worker, vapour}$	vapour concentration in air for workers	$[kg_c.m^{-3}]$	O
$C_{inh,worker, fibre}$	fibre concentration in air for workers	$[fibres.m^{-3}]$	O
$C_{inh,worker, dust}$	dust concentration in air for workers	$[kg_c.m^{-3}]$	O
$U_{der,pot,worker}$	potential dermal uptake rate for workers	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$U_{tot-v/d,worker}$	total uptake for one scenario via different routes	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$HT25worker_{inh,vapour,nt}$	human equivalent dose inhalatory worker vapour exposure, non-thr.	$[kg_c.m^{-3}]$	O
$HT25worker_{inh,fibr,nt}$	human equivalent dose inhalatory worker fibre exposure, non-thr.	$[fibres.m^{-3}]$	O
$HT25worker_{inh,dust,nt}$	human equivalent dose inhalatory worker dust exposure, non-thr.	$[kg_c.m^{-3}]$	O
$HT25worker_{der,nt}$	human equivalent dose dermal worker exposure, non-thr.	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$HT25worker_{tot-v/d,nt}$	human equivalent dose total worker exposure, non-thr.	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
CF_{occup2}	correction factor for duration and frequency of exposure	[-]	D

Output

$cLRcons_{inh,vaour,nt}$	lifetime cancer risk, inhalatory worker vapour exposure, non-thr.	[-]	O
$cLRcons_{inh,fibre,nt}$	lifetime cancer risk, inhalatory worker fibre exposure, non-thr.	[-]	O
$cLRcons_{inh,dust,nt}$	lifetime cancer risk, inhalatory worker dust exposure, non-thr.	[-]	O
$cLRcons_{der,nt}$	lifetime cancer risk, dermal worker exposure, non-thr.	[-]	O
$cLRcons_{tot,nt}$	lifetime cancer risk, total worker exposure, non-thr.	[-]	O

B. Margin Of Exposure

Calculation of scenario-specific MOE

Under the assumption that man is exposed throughout his or her lifetime, exposure of workers to a substance is compared to the T25 or CED (BMD05), resulting in a Risk Characterisation Ratio (RCR) called the Margin Of Exposure. This comparison is made for all relevant routes of exposure.

Depending on the available data the following RCRs are possible:

Effects / Exposure	**Exposure**	**Available effects data**
$MOEworker_{inh,vapour,nt}$	$C_{inh,worker,vapour}$ .1/CF_{occup2}	$T25_{mammal,inh,nt}$ $CED_{mammal,inh,nt}$
$MOEworker_{inh,fibre,nt}$	$C_{inh,worker,fibre}$ .1/CF_{occup2}	$T25_{mammal,inh,fibre,nt}$ $CED_{mammal,inh,fibre,nt}$
$MOEworker_{inh,dust,nt}$	$C_{inh,worker,dust}$.1/CF_{occup2}	$T25_{mammal,inh,dust,nt}$ $CED_{mammal,inh,,dust,nt}$
$MOEworker_{der,nt}$	$U_{der,pot,worker}$.1/CF_{occup2}	$T25_{mammal,der,nt}$ $CED_{mammal,der,nt}$
$MOEworker_{tot-v/d,nt}$	$U_{tot-v/d,worker}/(BIO_{oral,2}\ .\ CF_{occup2})$	$T25_{mammal,oral,nt}$ $CED_{mammal,oral,nt}$

Input			
$T25_{mammal,inh,,nt}$	inhalatory T25 for mammals for non-threshold effects	$[kg_c.m^{-3}]$	S/O
$T25_{mammal,inh,fibre,nt}$	inhalatory T25 (fibre)for mammals for non-threshold effects	$[fibres.m^{-3}]$	S/O
$T25_{mammal,inh,dust,nt}$	inhalatory T25 (dust) for mammals for non-threshold effects	$[kg_c.m^{-3}]$	S/O
$CED_{mammal,inh,nt}$	inhalatory CED for mammals for non-threshold effects	$[kg_c.m^{-3}]$	S/O
$CED_{mammal,inh,fibre,nt}$	inhalatory CED (fibe) for mammals for non-threshold effects	$[fibres.m^{-3}]$	S/O
$CED_{mammal,inh,dust,nt}$	inhalatory CED (dust) for mammals for non-threshold effects	$[kg_c.m^{-3}]$	S/O
$T25_{mammal,der,nt}$	dermal T25 for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,der,nt}$	dermal CED for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$C_{inh,worker, vapour}$	vapour concentration in air for workers	$[kg_c.m^{-3}]$	O
$C_{inh,worker, fibre}$	fibre concentration in air for workers	$[fibres.m^{-3}]$	O
$C_{inh,worker, dust}$	dust concentration in air for workers	$[kg_c.m^{-3}]$	O
$U_{der,,pot,worker}$	potential dermal uptake rate for workers	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$U_{tot-v/d,worker}$	total uptake for one scenario via different routes	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$BIO_{oral,2}$	bioavailability for oral uptake, starting route	[-]	D
CF_{occup2}	correction factor for duration and frequency of exposure	[-]	D
Output			
$MOEworker_{inh,vapour,nt}$	MOE inhalatory worker vapour exposure, non-thr.	[-]	O^c
$MOEworker_{inh,fibre,nt}$	MOE inhalatory worker fibre exposure, non-thr.	[-]	O^c
$MOEworker_{inh,dust,nt}$	MOE inhalatory worker dust exposure, non-thr.	[-]	O^c
$MOEworker_{der,nt}$	MOE dermal worker exposure, non-thr.	[-]	O^c
$MOEworker_{tot-v/d,nt}$	MOE total worker exposure, non-thr.	[-]	O^c

Derivation of scenario-specific reference-MOE

In order to account for the various uncertainties and variabilities in the extrapolation from experimental data to the worker situation and in the available data set, per scenario under consideration a reference-MOE is to be derived. All aspects that can be dealt with quantitatively (as assessment factors) are combined to form the overall assessment factor or reference-MOE (RMOE).

$$RMOEworker_{x,nt} = AF_{inter} \cdot AF_{allom} \cdot AF_{exprt} \cdot AF_{dose-resp} \cdot AF_{lr} .CF_{occup1} \quad \textbf{(884)}$$

$x \in$ {inh-vapour,inh-fibre, inh-dust, der,tot-v/d}

Input			
AF_{inter}	assessment factor for interspecies differences	[-]	S/D
AF_{allom}	assessment factor for allometric scaling	[-]	S/D
AF_{exprt}	assessment factor for differences in exposure route	[-]	S/D
$AF_{dose-resp}$	assessment factor for dose-response relationship	[-]	S/D
AFlr	assessment factor for extrapolation to a low risk level	[-]	S/D
CF_{occup1}	correction factor for respiratory rate in route-to-route extrapolation	[-]	S/D
Output			
$RMOEworker_{inh,vapour,nt}$	reference-MOE inhalatory worker vapour exposure, non-thr.	[-]	O^c
$RMOEworker_{inh,fibre,nt}$	reference-MOE inhalatory worker fibre exposure, non-thr.	[-]	O^c
$RMOEworker_{inh,dust,nt}$	reference-MOE inhalatory worker dust exposure, non-thr.	[-]	O^c
$RMOEworker_{der,nt}$	reference-MOE dermal worker exposure, non-thr.	[-]	O^c
$RMOEworker_{tot,nt}$	reference-MOE total worker exposure, non-thr.	[-]	O^c

For the route-to-route extrapolation for workers involving the inhalatory route an additional correction is used to account for the difference between the respiratory rate of the general population (default 20 m3 per 24 hrs) used in the route-to-route extrapolation and the respiratory rate of workers (10 m3 in 8 hrs). The TGD recommends a factor of 0.5 for extrapolations from the dermal and oral route to the inhalatory route and 2 for extrapolations from the inhalatory route to the dermal and oral route. EUSES allows this correction in the derivation of the RMOS, RMOE and human equivalent dose for workers. The default is 1.

Comparison of MOE with reference-MOE

The MOE is compared to the reference-MOE, resulting in a MOE/reference-MOE ratio (MRR).

Depending on the available data the following MRRs are possible:

RCR / reference-MOS	**RCR**	**Reference-MOS**
$MRRworker_{inh,vapour,nt}$	$MOEworker_{inh,vapour,nt}$	$RMOEworker_{inh,vapour,nt}$
$MRRworker_{inh,fibre,nt}$	$MOEworker_{inh,fibre,nt}$	$RMOEworker_{inh,fibre,nt}$
$MRRworker_{inh,dust,nt}$	$MOEworker_{inh,dust,nt}$	$RMOEworker_{inh,dust,nt}$
$MRRworker_{der,nt}$	$MOEworker_{der,nt}$	$RMOEworker_{der,nt}$
$MRRworker_{tot\text{-}v/d,nt}$	$MOEworker_{tot\text{-}v/d,nt}$	$RMOEworker_{tot\text{-}v/d,nt}$

Input

$MOEworker_{inh,vapour,nt}$	MOE inhalatory worker vapour exposure, non-thr.	[-]	O^c
$MOEworker_{inh,fibre,nt}$	MOE inhalatory worker fibre exposure, non-thr.	[-]	O^c
$MOEworker_{inh,dust,nt}$	MOE inhalatory worker dust exposure, non-thr.	[-]	O^c
$MOEworker_{der,nt}$	MOE dermal worker exposure, non-thr.	[-]	O^c
$MOEworker_{tot\text{-}v/d,nt}$	MOE total worker exposure, non-thr.	[-]	O^c
$RMOEworker_{inh,vapour,nt}$	reference-MOE inhalatory worker vapour exposure, non-thr.	[-]	O^c
$RMOEworker_{inh,fibre,nt}$	reference-MOE inhalatory worker fibre exposure, non-thr.	[-]	O^c
$RMOEworker_{inh,dust,nt}$	reference-MOE inhalatory worker dust exposure, non-thr.	[-]	O^c
$RMOEworker_{der,nt}$	reference-MOE dermal worker exposure, non-thr.	[-]	O^c
$RMOEworker_{tot,nt}$	reference-MOE total worker exposure, non-thr.	[-]	O^c

Output

$MRRworker_{inh,vapour,nt}$	ratio MOE/RMOE, inhalatory worker vapour exposure, non-thr.	[-]	O^c
$MRRworker_{inh,fibre,nt}$	ratio MOE/RMOE, inhalatory worker fibre exposure, non-thr.	[-]	O^c
$MRRworker_{inh,dust,nt}$	ratio MOE/RMOE, inhalatory worker dust exposure, non-thr.	[-]	O^c
$MRRworker_{der,nt}$	ratio MOE/RMOE, dermal worker exposure, non-thr.	[-]	O^c
$MRRworker_{tot\text{-}v/d,nt}$	ratio MOE/RMOE, total worker exposure, non-thr.	[-]	O^c

III.7.2.3.3 Derivation of AOEL for biocides with a threshold

Risk characterisation of biocides should be performed by the MOS-approach as well by comparing the AOEL to the internal operator/bystander exposure values of corresponding time scale, resulting in a AOEL/exposure ratio (AER). The MOS-approach has already been described above. This section describes the default AOEL-procedure in EUSES.
Exposure estimated for biocides can be derived by measuring and by the application of various models. EUSES offers the possibility to use the TGD-consumer exposure models or to enter monitoring data. The EASE model results are generally not applicable to biocides since the scenarios relate to industrial use of chemicals. Other models may be used and the relevant exposure results entered in EUSES.

Derivation of AOEL and reference-MOS

As default-procedure, the AOEL (Acceptable Operator Exposure Level) is based on the NOAEL (or exceptionally, LOAEL) from an oral short-term toxicity study (28- or 90-day study), which is to be converted to an internal dose by correction for systemic bioavailability. EUSES also performs the AOEL procedure on the basis of inhalatory and dermal N(L)OAELs from short-term toxicity studies. If both an N(L)OAEL for man and an N(L)OAEL for mammals are available, the former one is used. The user may decide to deviate from the default procedure and to base the AOEL on a NOAEL from other studies than the 28- or 90-day study. The internal N(L)OAEL is then divided by the overall assessment factor or reference-MOS (RMOS), to

$$\boldsymbol{RMOSaoel_{x,y} = AF_{inter} \cdot AF_{allom} \cdot AF_{intra} \cdot AF_{expdur} \cdot AF_{exprt} \cdot AF_{dose-resp} \cdot CF_{occup1}} \quad \mathbf{(885)}$$

account for uncertainties in the extrapolation from experimental data to the human situation.

$x \in$ {oral,inh,der}
$y \in$ {repdose, fert,carc} (repdose is default)

Input			
AF_{allom}	assessment factor for allometric scaling	[-]	S/D
AF_{inter}	assessment factor for remaining interspecies differences	[-]	S/D
AF_{intra}	assessment factor for intraspecies differences	[-]	S/D
AF_{expdur}	assessment factor for differences in exposure duration	[-]	S/D
AF_{exprt}	assessment factor for differences in exposure route	[-]	S/D
$AF_{dose-resp}$	assessment factor for dose-response relationship	[-]	S/D
AF_{nature}	assessment factor for nature of effect	[-]	S/D
AF_{data}	assessment factor for adequacy of/confidence in database	[-]	S/D
CF_{occup1}	correction factor for respiratory rate in route-to-route extrapolation	[-]	S/D
Output			
$RMOSaoel_{oral,y}$	reference-MOS oral exposure for endpoint y	[-]	O^c
$RMOSaoel_{inh,,y}$	reference-MOS inhalatory exposure for endpoint y	[-]	O^c
$RMOSaoel_{der,y}$	reference-MOS dermal exposure for endpoint y	[-]	O^c

If only a N(L)OAEL for mammals is available:

$$\boldsymbol{AOEL_{1,x} = \frac{N(L)OAEL_{mammal,x,y} \cdot BIO_{x,2}}{RMOSaoel_{x,y}}} \quad \mathbf{(886)}$$

If a N(L)OAEL for man is available:

$$\boldsymbol{AOEL_{2,x} = \frac{N(L)OAEL_{man,x,y} \cdot BIO_{x,2}}{RMOSaoel_{x,y}}} \quad \mathbf{(887)}$$

$x \in$ {oral,inh,der}

$y \in$ {repdose, fert,carc} repdose is default

Input

$N(L)OAEL_{mammal,oral,y}$	oral N(L)OAEL for mammals for endpoint y	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$N(L)OAEL_{mammal,inh,y}$	inhalatory N(L)OAEL for mammals for endpoint y	$[kg_c.m^{-3}]$	S/O
$N(L)OAEL_{mammal,der,y}$	oral N(L)OAEL for mammals for endpoint y	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$N(L)OAEL_{man,oral,y}$	oral N(L)OAEL for man for endpoint y	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$N(L)OAEL_{man,inh,y}$	inhalatory N(L)OAEL for man for endpoint y	$[kg_c.m^{-3}]$	S/O
$N(L)OAEL_{man,der,y}$	dermal N(L)OAEL for man for endpoint y	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$BIO_{oral,2}$	bioavailability for oral uptake (end route)	[-]	S/D
$BIO_{inh,2}$	bioavailability for inhalatory uptake (end route)	[-]	S/D
$BIO_{der,2}$	bioavailability for dermal uptake (end route)	[-]	S/D
$RMOSaoel_{oral,,y}$	reference-MOS oral exposure for endpoint y	[-]	O^c
$RMOSaoel_{inh,,y}$	reference-MOS inhalatory exposure for endpoint y	[-]	O^c
$RMOSaoel_{der,y}$	reference-MOS dermal exposure for endpoint y	[-]	O^c

Output

$AOEL_{1,oral}$	AOEL, based on oral study in mammals	$[kg.kg_{bw}^{-1}.d^{-1}]$	O^c
$AOEL_{1,inh}$	AOEL, based on inhalatory study in mammals	$[kg_c.m^{-3}]$	O^c
$AOEL_{1,der}$	AOEL, based on dermal study in mammals	$[kg.kg_{bw}^{-1}.d^{-1}]$	O^c
$AOEL_{2,oral}$	AOEL, based on oral study in man	$[kg.kg_{bw}^{-1}.d^{-1}]$	O^c
$AOEL_{2,inh}$	AOEL, based on inhalatory study in man	$[kg_c.m^{-3}]$	O^c
$AOEL_{2,der}$	AOEL, based on dermal study in man	$[kg.kg_{bw}^{-1}.d^{-1}]$	O^c

2. Comparison of AOEL with exposure

Depending on the available data the following AERs are possible:

AOEL / Exposure	**AOEL**	**Exposure**
$AER_{1,oral}$	$AOEL_{1,oral}$	$I_{oral} . BIO_{oral,2}$
$AER_{1,inh}$	$AOEL_{1,inh}$	$I_{inh} \cdot BIO_{inh,2}$
$AER_{1,der}$	$AOEL_{1,der}$	$U_{der,pot} \cdot BIO_{der,2}$
$AER_{1,tot}$	$AOEL_{1,oral}$	U_{tot}
$AER_{2,oral}$	$AOEL_{2,oral}$	$I_{oral} . BIO_{oral,2}$
$AER_{2,inh}$	$AOEL_{2,inh}$	$I_{inh} \cdot BIO_{inh,2}$
$AER_{2,der}$	$AOEL_{2,der}$	$U_{der,pot} \cdot BIO_{der,2}$
$AER_{2,tot}$	$AOEL_{2,oral}$	U_{tot}

Input

$AOEL_{1,oral}$	AOEL, based on oral study in mammals	$[kg.kg_{bw}^{-1}.d^{-1}]$	O^c
$AOEL_{1,inh}$	AOEL, based on inhalatory study in mammals	$[kg_c.m^{-3}]$	O^c
$AOEL_{1,der}$	AOEL, based on dermal study in mammals	$[kg.kg_{bw}^{-1}.d^{-1}]$	O^c
$AOEL_{2,oral}$	AOEL, based on oral study in man	$[kg.kg_{bw}^{-1}.d^{-1}]$	O^c
$AOEL_{2,inh}$	AOEL, based on inhalatory study in man	$[kg_c.m^{-3}]$	O^c
$AOEL_{2,der}$	AOEL, based on dermal study in man	$[kg.kg_{bw}^{-1}.d^{-1}]$	O^c
I_{oral}	ingestion rate of substance	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
I_{inh}	inhalatory intake of substance	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$U_{der,pot}$	amount of substance that potentially can be taken up	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
U_{tot}	total uptake via different routes	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$BIO_{oral,2}$	bioavailability for oral uptake (end route)	[-]	S/D
$BIO_{der,2}$	bioavailability for dermal uptake (end route)	[-]	S/D
$BIO_{inh,2}$	bioavailability for inhalation (end route)	[-]	S/D

Output

$AER_{1,oral}$	ratio oral $AOEL_1$ / internal oral exposure	[-]	O^c
$AER_{1,inh}$	ratio inhalatory $AOEL_1$ / internal inhalator exposure	[-]	O^c
$AER_{1,der}$	ratio dermal $AOEL_1$ / internal dermal y exposure	[-]	O^c
$AER_{1,tot}$	ratio oral $AOEL_1$ / internal total exposure	[-]	O^c
$AER_{2,oral}$	ratio oral $AOEL_2$ / internal oral exposure	[-]	O^c
$AER_{2,inh}$	ratio inhalatory $AOEL_2$/ internal inhalatory exposure	[-]	O^c
$AER_{2,der}$	ratio dermal $AOEL_2$ / internal dermal exposure	[-]	O^c
$AER_{2,tot}$	ratio oral $AOEL_2$ / total internal exposure	[-]	O^c

III.8 HYDROCARBON BLOCK METHOD (HBM)

The principal steps in the application of the Hydrocarbon Block Method (HBM) are:

- obtain compositional data for the substance that are sufficient to assign components to blocks;
- define blocks by grouping components on the basis of similar structural and/or physico-chemical and ecotoxicological properties. If desired, blocks can be defined as single components;
- obtain production and use data;
- establish release estimates for each block. A single release estimate for a petroleum substance may not always be adequate; blocks with markedly different physico-chemical properties may require different release estimates;
- assign representative values for physico-chemical properties, degradation-rate constants and LC/EC50s and NOECs to each block;
- determine the PEC for each compartment for each block (local as well as regional);
- determine the PNEC for each block;
- calculate the PEC/PNEC ratio for each block, and sum.

Once the blocks with their physico-chemical and ecotoxicological properties have been defined, the assessment follows the methods described in the following sections. This means that local and regional PECs can be calculated as described in the 'Environmental distribution module' and a PNEC can be derived as described in the 'Effects assessment module'.

III.9 ENVIRONMENTAL RISK ASSESSMENT FOR METALS AND METAL COMPOUNDS

In principle, the models and approaches for organic substances can also be used to estimate exposure to metals. However, there are several differences compared with the use of these models for organic substances. Below, the differences are described.

III.9.1 Exposure assessment

1. *Physico-chemical properties (Input module)*

In general, water solubility, boiling point and vapour pressure cannot be used. The octanol-water partition coefficient is not appropriate and measured partition coefficients (*Kp*) should be used instead.

2. *Partition coefficients (Environmental distribution module, partition coefficients sub-module)*

Adsorption to aerosol particles

Most of the metal present in the atmosphere will be bound to aerosols. Therefore, an extremely low value for the vapour pressure should be used to estimate the fraction bound to aerosol, e.g. 10^{-20} Pa. This leads to a value for $Fass_{aer}$ almost equal to one. If a valid measured value is available for the aerosol-bound fraction, this value can be used.

Volatilisation

Volatilisation can be ignored for metals, except for mercury compounds and several organometallo-compounds. Therefore, the Henry coefficient should generally be set to a very low value.

Adsorption/desorption

Formulae to estimate *Koc* cannot be used. Measured *Kp*-values must be used for water-soil, water-sediment and water-suspended matter. *Kp* is influenced by speciation and the speciation behaviour must therefore be accounted for in *Kp*.

3. *Biotic and abiotic degradation rates (Environmental distribution module, Environmental degradation rates sub-module)*

Not relevant for metals. The substances must be specified as non-biodegradable (very high DT50).

4. *Elimination processes prior to the release in the environment (Environmental distribution module, Sewage treatment sub-module)*

For applying the STP model, a partition coefficient is used for water-sludge. For metals, a measured *Kp*-value must be used.

5. *Calculation of the regional PEC (Environmental distribution module, Regional environmental distribution sub-module)*

The values applied for model parameters for the regional model, inter-media mass-transfer coefficients and model parameters for the continental concentration can be used.

III.9.2 Effects assessment

PNECs can be derived through the application of assessment factors on the basis of the available data. Evaluation of the toxicity data is critical (the reader is referred to the TGD; EC, 1996). Standard methods applied for organic compounds can be used for this (see Section III.6). However, because of the specific mode of action that metals may have for some species, care should be taken in extrapolating short term toxicity data to the PNEC using the standard assessment factors. For many metals, sufficient long term toxicity data for aquatic organisms may be present to enable statistical extrapolation, results of which can support the results of PNECs calculated using assessment factors. Calculated PNECs derived for essential metals may not be lower than natural background concentrations.

A prerequisite for the derivation of the PNEC is that it is done on the basis of the same level of availability as in exposure assessment:
- Results from aquatic toxicity tests are usually expressed as total concentrations. As a first approach, total concentrations have to be recalculated to dissolved concentrations using partition coefficients. If this is not possible, the total concentration can be set equal to the dissolved concentration. Differences in test systems, e.g. (semi-)static versus continuous flow systems and natural versus standard water, have to be considered.
- For the terrestrial compartment, many data exist, but most are only expressed as total concentration that has been added to the test media. This added amount will be partitioned among the aqueous and the solid phase. Application of partition coefficients to calculate the available concentration in soil can be applied. Soil type correction, using reference lines, should be applied to correct for differences among soil types (Slooff, 1992).
- Some of the metals are essential metals, having a function in biological processes at low concentrations. Shortage of micronutrients may cause malfunction. This implies that in setting the PNEC, information on deficiency levels should be taken into account. It should, however, be noted that often no information on deficiency levels of various metals for various species is available.

Though some exceptions exist, in general ionic metal species are considered to be the dominant metal species taken up, and are thus considered to be the metal species responsible for the toxic effect. Data on the concentration of ionic species in aquatic and terrestrial systems are not readily available, and cannot, as yet, be applied on a regular basis in risk assessment.

Bioaccumulation of essential metals
Metals are taken up by organisms. For essential metals, biota regulate their uptake by means of the general physiological mechanism of homeostasis. By this mechanism, organisms will keep, within a certain range of varying external concentrations, their intracellular levels relatively constant, in order to satisfy their requirements for that essential element. Homeostasis implies that organisms can actively concentrate essential elements if concentrations in the environment are very low. This may lead to high BCF values. On the other hand, the homeostatic regulation capacity will be exceeded at a given higher external concentration beyond which the element will accumulate and become toxic.