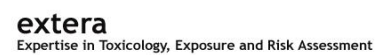




**CropLife Europe Guidance on REACH Chemical Safety Assessment for Co-Formulants Used  
in Crop Protection Products**

The REACH-IN Project

**April 2024**



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## Sector-Specific Terminology and Abbreviations

<b>Plant Protection Product Terminology</b>	<b>REACH Equivalent Terminology / Clarification</b>
AI	Active ingredient
PPP	Plant protection product
CPP	Crop protection product
Co-formulant	A component of a formulation other than the AI. Also sometimes referred to as an “inert”.
Formulation	Preparation or mixture
Farmer	Professional worker
Amateur	Consumer
Bystanders	Members of the public potentially exposed during application of a PPP
Re-entry	A situation in which a worker is entering an area after it has been treated with a PPP

### Disclaimer

CropLife Europe developed the CLE OWB and LET tools to enable users to perform human and local scale environmental exposure and risk assessments for substances used as co-formulants in plant protection products. The content of the spreadsheets within the tools must not be modified. The tools have been subjected to thorough testing; however, CLE does not guarantee that the tools work error-free. CLE offers no warranty either to the reliability of the tools and of the provided information or to the conclusions or assumptions made by any user on the basis of the use of these tools or the use of such information or to the regulatory acceptance of Chemical Safety Assessments conducted using the CLE OWB and LET. All usage is at the discretion of the user and CLE is not liable for any consequences resulting from such use.

## Introduction

In order to comply with the requirements of Regulation (EC) No. 1907/2006 (REACH), it is necessary to perform a chemical safety assessment for substances manufactured in or imported into the European Economic Area in quantities of equal to or greater than 10 tonnes/year. For substances meeting the criteria for classification under Regulation (EC) No. 1272/2008 (CLP), a quantitative (or qualitative) exposure assessment and risk characterisation will be required, covering all relevant identified uses of a substance.

Accordingly, CropLife Europe (CLE) has developed a standardised approach with regards to fulfilling this obligation for substances that are used as co-formulants in plant protection products (PPP).

The elements described in this document result from a project called REACH-IN. Further information can be found on the CropLife Europe website (<https://croplifeeurope.eu/resources/reach-in-registration-evaluation-authorisation-and-restriction-of-chemicals/>).

An exposure modelling tool (OWB) has been developed to assess the potential exposure of professional workers (i.e., farmers, licensed professional operators) and consumers to co-formulants arising from plant protection product uses. CLE OWB allows the exposure assessor to take account of risk management measures (RMM) such as personal protective equipment (PPE) and respiratory protective equipment (RPE) in the exposure estimation for professionals. The tool also provides the feature to automatically populate templates of the relevant sections of the chemical safety report (CSR).

For the purpose of the environmental risk assessment, a set of tools have been developed:

- CLE Specific Environmental Release Categories (SpERCs)
- CLE Local Environment Tool (CLE LET)

CLE SpERCs have been developed and are incorporated in the ECETOC TRA since version 2 (however, TRA version 3.1 uses previous versions of the SpERCs that have to be updated manually), but can also be utilised in Chesar, and “manually” in EUSES. The SpERCs are conservative and are recommended in a first-tier environmental risk assessment for the assessment of regional scale environmental exposure.

To complement the SpERCs, CLE has developed the LET for the specific assessment of potential exposure at the local scale, including secondary poisoning and indirect exposure of man via the environment, arising from plant protection product uses. The LET is a simple Excel-based tool, which should be used to replace the local scale calculations from ECETOC TRA, EUSES, Chesar, etc. Both SpERCs and LET, work in combination in order to cover all environmental exposures related to the use of substances as a co-formulant in PPP.

# 1. The CropLife Europe Generic Exposure Scenarios

## 1.1 Introduction

This section of the document provides an overview of the Identified Uses, Generic Exposure Scenarios and associated Use Descriptors considered being the minimum required to cover substances used as co-formulants in plant protection products (PPP).

Furthermore, it describes the link between the Use Descriptors and the activities covered in the REACH-IN exposure modelling tools developed by CLE. Further details on using the REACH-IN models can be found in later sections of this manual.

For a proper reading of this guidance, a good working knowledge of REACH and its terminology is assumed. The extensive REACH guidance provided by the European Chemicals Agency (ECHA) should be consulted for more details in this area.

In principle many different Tier 1, or higher-tier, models could be used to generate exposure estimates for the activities described in section 1.2. However, because of the specialised nature of the use pattern and exposure determinants in the agrochemical industry, CLE has developed tools (based on existing models already in use in the agrochemical industry and with regulatory acceptance) linked to the above scenarios suitable for use in REACH risk assessments. The use of these tools in the assessment of substances used as co-formulants in PPP is highly recommended.

The CLE OWB tool is used to assess worker and consumer exposure to co-formulants. The OWB is based on several different models which are used in parallel to assess the various sub-activities covered by CLE GES. These models thus define the scope (tasks and use patterns) for the worker and consumer contributing scenarios.

The CLE SpERCs and LET should be used to assess the environmental exposure, human exposure via the environment, and secondary poisoning.

The CLE REACH-IN tools are designed to provide output directly linked to the Identified Uses and Generic Exposure Scenarios. The following sections describe for each GES the tasks covered by each contributing scenario and Use Descriptor. In particular for the CLE OWB, these are defined by the underlying exposure models.

## 1.2 Identified Uses and Use Descriptor Assignment

An expert group assigned by the European Crop Protection Association (ECPA, now CropLife Europe) has summarised the identified uses of substances as co-formulants in PPP in four Generic Exposure Scenarios (Dobe et al., 2017). The CLE GES describe the common identified uses as co-formulants in PPP based on the use descriptor system developed by ECHA.

It is important to note that for co-formulant uses in PPP, the assignment of Use Descriptors is purely for ease of standard communication up and down the supply chain. As such, the default input parameters or exposure models generally used for a specific Use Descriptor for industrial or professional activities may not be appropriate (e.g., some Environmental Release Categories are not appropriate for the co-formulant use in PPP, and instead the CLE SpERCs and LET should be used).

A REACH risk assessment for a substance used as a co-formulant may be required for the following typical activities with PPP:

- mixing, loading and spraying of formulations
- treatment of seeds with formulations, handling and sowing of treated seeds
- handling and dispersion of granular formulations (direct application to soil).

These tasks have been summarised and collated into the following four Generic Exposure Scenarios and combinations of appropriate Use Descriptors (Dobe et al., 2017). While not necessarily covering



all possible application methods, the four GES are considered to cover the most common methods. Although not mandatory for professional uses, it is now recommended to include the Product Category (PC) ‘Pesticides (PC27)’ as a Use Descriptor.

### 1.2.1 Identified Uses

Each Identified Use has an associated Generic Exposure Scenario, which can be broken down by task (e.g., mixing and loading) into several contributing scenarios for workers (farmers, professional contractors), consumers and the environment.

<b>Professional Uses – Generic Exposure Scenario 1</b>		
Identified Use		Use as a co-formulant in plant protection products, spray applications by professionals
Short exposure scenario title		Use as a co-formulant in plant protection products, spray applications by professionals
Systematic use descriptors		PW, SU1, PROC 8a, PROC 11, PC27, CLE SpERC 8d.2.v4
Environment CS 1	CLE SpERC 8d.2.v4 (see Chapter 3.7)	Spray application of plant protection products containing co-formulants (indoor or outdoor)
Worker CS 2	PROC 8a (see Chapter 2.5.2.2)	Mixing and loading of plant protection products into delivery equipment
Worker CS 3	PROC 11 (see Chapter 2.5.2.3)	Delivery and dispersion of plant protection products

<b>Professional Uses – Generic Exposure Scenario 2</b>		
Identified Use		Use as a co-formulant in plant protection products, seed and granular applications by professionals
Short exposure scenario title		Use as a co-formulant in plant protection products, seed and granular applications by professionals
Systematic use descriptors		PW, SU1, PROC 8a, PROC 8b, PC27, CLE SpERC 8d.1.v4
Environment CS 1	CLE SpERC 8d.1.v4 (see Chapter 3.7)	Direct application of plant protection products (granules or treated seeds) containing co-formulants to soil (indoor or outdoor)
Worker CS 2	PROC 8a (see Chapter 2.5.3.2)	Mixing and loading of plant protection products into seed treatment or delivery equipment
Worker CS 3	PROC 8b (see Chapter 2.5.3.3)	Transfer of treated seeds from batch treater into bags
Worker CS 4	PROC 8a (see Chapter 2.5.3.4)	Delivery and dispersion of agrochemical plant protection products or treated seeds

<b>Consumer Uses – Generic Exposure Scenario 3</b>		
Identified Use		Use as a co-formulant in plant protection products, spray applications by consumers
Short exposure scenario title		Use as a co-formulant in plant protection products, spray applications by consumers
Systematic use descriptors		C, PC27, CLE SpERC 8d.2.v4
Environment CS 1	CLE SpERC 8d.2.v4 (see Chapter 3.7)	Spray application of plant protection products containing co-formulants (indoor or outdoor)
Consumer CS 2	PC27 (see Chapter 2.5.4.2)	Spray application of agrochemical plant protection products

<b>Consumer Uses – Generic Exposure Scenario 4</b>		
Identified Use		Use as a co-formulant in plant protection products, seed and granular applications by consumers
Short exposure scenario title		Use as a co-formulant in plant protection products, seed and granular applications by consumers
Systematic use descriptors		C, PC27, CLE SpERC 8d.1.v4
Environment CS 1	CLE SpERC 8d.1.v4 (see Chapter 3.7)	Direct application of plant protection products (granules or treated seeds) containing co-formulants to soil (indoor or outdoor)
Consumer CS 2	PC27 (see Chapter 2.5.5.2)	Manual spreading of granular plant protection products or treated seeds

Further activities related to smaller scale application methods, such as painting, fogging, dusting, and dipping, while not included above, are likely to fall either within the scope of generic exposure scenarios describing the use of substances in mixtures and formulations, and as such may not warrant an agrochemical-sector specific exposure scenario or are niche applications.

## 1.2.2 Use Descriptor Entry in IUCLID 6

The following examples are for Use Descriptor entry in IUCLID 6 (version 7.0.4) Section 3.5.

### Use by Professional Workers

Contributing activity / technique for the environment  New item 

**1** **Name of activity / technique**  
 Spray application of plant protection products containing co-formulants (indoor or outdoor)

**Environmental release category (ERC)**  
 ERC8d: Widespread use of non-reactive processing aid (no inclusion into or onto article, outdoor)

Contributing activity / technique for workers  New item 

**1** **Name of activity / technique**  
 Mixing and loading of plant protection products into delivery equipment

**Process category (PROC)**  
 PROC 8a: Transfer of substance or mixture (charging and discharging) at non-dedicated facilities

**2** **Name of activity / technique**  
 Delivery and dispersion of plant protection products

**Process category (PROC)**  
 PROC 11: Non industrial spraying

**Product category used**

PC 27: Plant protection products

**Sector of end use**

SU 1: Agriculture, forestry and fishing

**Technical function of the substance during use**

None

**Substance supplied to that use in form of**

in a mixture

## Consumers Uses

Contributing activity / technique for the environment + New item

**1 Name of activity / technique**  
Direct application of plant protection products (granules or treated seeds) containing co-formulants to soil (indoor or outdoor)

**Environmental release category (ERC)**  
✓ ERC8d: Widespread use of non-reactive processing aid (no inclusion into or onto article, outdoor)

Contributing activity / technique for consumers + New item

**1 Name of activity / technique**  
Manual spreading of granular plant protection products or treated seeds

**Product category (PC)**  
✓ PC 27: Plant protection products

Technical function of the substance during use

None

Substance supplied to this use in the form of

✓ in a mixture

### 1.2.3 Previous Identified Use Compilations

An earlier compilation of Use Descriptors made available by ECPA contained a total of 14 Identified Uses for co-formulants in PPP (*ECPA\_reach\_in\_Use\_Descriptors\_comp.doc*). These have been consolidated and simplified by recognising the common tasks inherent to each use. This leads to the four GES now described, and the resulting advantage of more efficient Downstream User communication. There is no change in the extent of the Identified Use coverage.

The Identified Uses previously listed for Professional Uses were:

- Co-formulant in plant protection products for outdoor spraying
- Co-formulant in plant protection products for indoor spraying
- Application of pre-treated seeds (outdoors)
- Application of pre-treated seeds (indoors)
- Co-formulant in plant protection products for seed treatment (outdoors)
- Co-formulant in plant protection products for seed treatment (indoors)
- Application of granular formulations using automated system (outdoors)
- Application of granular formulations using automated system (indoors)

The Identified Uses for Consumer Uses were:

- Co-formulant in plant protection products for outdoor spraying
- Co-formulant in plant protection products for indoor spraying
- Application of pre-treated seeds (outdoors)
- Application of pre-treated seeds (indoors)
- Application of granular formulations (outdoors)
- Application of granular formulations (indoors).

### **1.2.4 Separation of Contributing Scenarios**

On a case-by-case basis it may be necessary to further separate the communicated contributing scenarios for greater clarity, and to allow better differentiation of RMM. For example, where RMM are required, constraints within SDS authoring software may dictate that PROC 11 of PPP GES1 (Use as a co-formulant in plant protection products, spray applications by professionals) must be split into separate tractor and hand-held spraying scenarios. Such a constraint could arise from standard phrases and an inability to indicate which activity required the RMM, e.g., use of RPE for hand-held spraying only. Creating two PROC 11 contributing scenarios for PPP GES1 and splitting the exposure estimation table generated by the OWB tool appropriately between the two, would provide a simple solution.

The default combined PROC 11 is preferred where this differentiation is not needed, as it creates the most compact and efficient exposure scenarios for communication, i.e., the shortest CSR and annex to the SDS.

### **1.2.5 Scaling**

It is recommended that the following text be modified as appropriate and incorporated into section 4 of the exposure scenarios communicated to Downstream Users via the SDS:

“The above exposure scenario may be scaled using the CLE OWB tool (version 5.0) and using the parameters: application rate, personal protection (PPE), respiratory protection (RPE), and local exhaust ventilation (LEV).”

“The above exposure scenario may be scaled using the CLE Local Environment Tool (version 4.0) and using the parameters: co-formulant application rate, number of applications, application interval, crop (drift rate), location and period of application.”

## **2 Human health: The CLE Exposure Tool for Operators, Workers and Bystanders (CLE OWB)**

### **2.1 Introduction**

The sector-specific CLE OWB tool has been developed for the assessment of the potential exposure of operators, workers, and bystanders to co-formulants contained in plant protection products (PPP). OWB can be used to assess the exposure of professional workers (farmers, professional contractors) and consumers during mixing and loading activities, the spray application of products and dispersion of granular products or treated seeds. OWB is largely based on specific exposure models that were designed for the authorisation of plant protection products in Europe. These models have been developed from dosimetry studies that were conducted during actual field applications of PPP. OWB therefore provides a realistic depiction of the actual exposure situation compared to other screening tools, such as ECETOC TRA, which lack parameters specific for applications of PPP. In addition, OWB allows the user to take account of RMM such as personal or respiratory protective equipment (PPE, RPE) in the exposure estimation. The tool also provides the facility to automatically populate templates of the relevant sections of the CSR and generate the relevant exposure scenarios for the co-formulant use of a substance in PPP.

Sections 2.2 to 2.4 cover use of the OWB software. Section 2.5 describes the detailed methodology and algorithms used.

### **2.2 General Requirements**

- CLE OWB will run under MS EXCEL 2010 and higher versions.
- Macros must be allowed after start
- In order to generate output files using decimal points rather than commas, the regional setting within WINDOWS must be set to an English number format.

- The working directory containing the EXCEL file must contain a folder named "Templates" containing the three MS WORD files (templates)
  - CSR-9-10.docx
  - Summary.docx
  - GES Report.docx
- Use the "Save As" command to save the EXCEL file for documentation of model runs.

### **2.3 *Version history***

- V1.0 (April 2010)
- V2.1 (April 2012)
  - Introduction of granular application scenarios
- V2.2 (May 2012)
  - Secondary scenarios have been removed from the "Input & Report" screen
  - Button for exporting PPP GES sheets into a WORD file has been created
  - Renaming of GES sheets
- V2.3 (July 2012)
  - Extension of Mixing & Loading scenarios to additional formulation types
  - Inclusion of additional scenario for granular application by amateurs
  - Re-structuring of CSR Chapter 9 output
- V2.4 (January 2013)
  - The vapour exposure model in greenhouses was changed to a vapour pressure cut-off of 0.1 Pa. No vapour exposure below this cut-off; instantaneous release above the cut-off.
  - Molecular Weight input is not required anymore
  - Foliar residues at time of re-entry are zero for substances with a vapour pressure of 0.1 Pa or higher.
  - Re-structuring of CSR Chapter 9 output
- V2.5 (April 2013)
  - Worst-case scenario for tractor-mounted spraying changes from boom spraying to air-blast if gloves are worn.
- V2.6 (February 2014)
  - The CSR template has been adapted to the latest CSR template of ECHA (December 2013)
  - The method for determining the worst-case scenarios for each sub-activity has been refined to accommodate certain combinations of DNELs and PPE
- V3.0 (June 2014)
  - Integration of the CSR template for LET into the CSR template of OWB
- V3.1 (November 2014)
  - Introduction of a case selection for solid or liquid co-formulants. Liquid co-formulants will not be used in solid viz. dusty PPPs, so that an unnecessary over-prediction of inhalation during M&L is avoided
  - More queries are introduced to ensure that the worst-case is selected even for unlikely combinations of PPE, use rate, and DNELs
  - The 'bagging' scenario has been modified so that only ECETOC TRA default parameters for exposed skin surface and glove penetration are employed
- V3.2 (February 2015)
  - Generates outputs in .docx format
  - Hand surface of consumers is 840 cm<sup>2</sup> instead of 960 cm<sup>2</sup> for workers, in alignment with REACH GD R.15
  - CSR Format now based on the ECHA template implemented in IUCLID 5.6
  - Macro buttons now implemented as Form Buttons, not ActiveX controls for better version-to-version stability
- V3.3 (October 2015)

- Fixed a situation that allowed bystander RCRs to exceed 1 after using the maximisation function
- V4.0 (October 2016)
  - The underlying exposure models were changed from the “German model” to the updated Agricultural operator exposure model (AOEM; EFSA, 2014), where applicable. Accordingly, residents are now included as exposed population.
  - In accordance with ECPA Good Practices, wearing of gloves during M&L and seed/granular applications is considered the standard PPE, and thus applied by default.
  - Seed treatment has been removed from the OWB tool, pending the release of the currently ongoing development of a dedicated model for the estimation of operator exposure during seed treatment
- V4.1 (July 2021)
  - An error in the RCR calculation formula for PPR GES2 has been fixed. The predicted safe application rate for the professional use of granules and treated seeds is lowered to some extent as a result of this change. Risk assessors are advised to repeat the risk assessment for the professional use of a co-formulant applied as granular formulation or treated seeds.
  - An error in the calculation of vapour drift exposure has been fixed. This change leads to a minor increase in the predicted inhalation exposure of by-standers, which is not anticipated to impact the predicted safe application rate for spray application.
  - RCRs are calculated for all routes/populations for which a DNEL is entered.
  - If hand-held uses are not foreseen, the respective application rate can be set to zero and secondary exposure will be calculated for the tractor-mounted use only.
  - Exposure to spray and vapour drift is considered for workers only (linked to assessment of short-term residential exposure in separate tab).
  - Short-term residential exposure via drift and surface deposits was moved to a separate tab for ad hoc assessments because of the mismatch in duration with chronic DNELs used in the standard assessment
  - TCs for crop-type "General" are used as default for re-entry workers.
  - Upwards or downwards hand-held spraying are carried forward to risk assessment, depending on which gives the worst-case combined RCR.
  - Bugs fixed:
    - CRRM calculations were not correctly implemented in the indoor hand-held spraying scenario. The correction resulted in a minimal increase in the predicted inhalation exposure, which had not impact on the estimated safe application rate.
    - Belly grinder dermal exposure data were not correctly fed into the PPP GES 4 calculations. The correction resulted in a lower safe application rate for the consumer use of granular formulations and treated seeds. Risk assessors are advised to repeat the risk assessment for the consumer use of a co-formulant applied as granular formulation or treated seeds.
  - Hand exposure during manual application of granules was modified to match the EFSA AOEM approach (gloves PF 100).
- V5.0 (December 2023)
  - Implementation of the updated EFSA Guidance (EFSA, 2022)
    - Updated equations for operator exposure according to guidance
    - Implementation of the new EFSA model for indoor spraying
    - Update of anthropometric parameters
    - Revised list of crops and re-entry transfer coefficients

## 2.4 User guidance

### 2.4.1 Inputs

All user input takes place on the "Input & Report" sheet.

Only the white cells can be edited. Some cells contain helpful comments. Move the cursor over the red triangles in the upper right-hand corner of the cells to make the comments visible.

**(1) Identifier**

A substance name and an optional identifier can be entered. These inputs will form the CSR file names.

If you do not change either identifier between assessments, the previous file will be overwritten.

**(2) Substance Data**

- Vapour pressure (Pa) and molecular weight (g/mol) must be entered
- Physical state of the co-formulant. If "liquid", certain scenarios pertaining to dusty formulations will not apply

Substance	
<b>Substance data</b>	
Vapour pressure (room temp.)	Pa
Molecular weight	g/mol
Physical state (room temp.)	solid
<b>DNELs</b>	
Worker, long term, inhalation	mg/m <sup>3</sup>
Worker, long term, dermal	mg/kg bw /day
General population, long term, inhalation	mg/m <sup>3</sup>
General population, long term, dermal	mg/kg bw /day

**(3) Hazard Data (necessary for Risk Characterisation)**

- inhalation and dermal DNELs for workers must be entered using the appropriate units
- inhalation and dermal DNELs for the general population must be entered using the appropriate units

**Systemic or local DNELs (pull-down menu)**

- Dermal DNELs must be entered in mg/kg bw/day if based on systemic effects (default)
- Dermal DNELs must be entered in mg/cm<sup>2</sup> if based on local effects (irritation/corrosion, sensitisation).



### 2.4.2 Scenario information

Scenario information	ES no.	Professional uses					
		PPP GES1 Spray application			PPP GES2 Seed and granular application	PPP GES3	PPP GES4
ES sub-activity		Tractor-mounted spraying	Hand-held spraying, outdoor	Hand-held spraying, indoor	Dispersing granules/ seeds	Hand-held spraying, indoor	Dispersing granules/ seeds
Application rate (kg/ha)		1.00	<b>0.500</b>	1.00	20.0	1.00	20.0
Personal protection (PPE)		Gloves M&L	Gloves M&L	Gloves M&L	Work wear + gloves		
Respiratory protection (RPE)		no RPE	no RPE	no RPE	no RPE		

Application rates can be entered (only numerical values). Smaller-than-default application rates will appear in bold font

ES # as it appears in the CSR

Various degrees of PPE and RPE are available from dropdown menus (default is "Gloves M&L"). Coverall and RPE will appear in bold font

PPE/RPE is not available for consumers

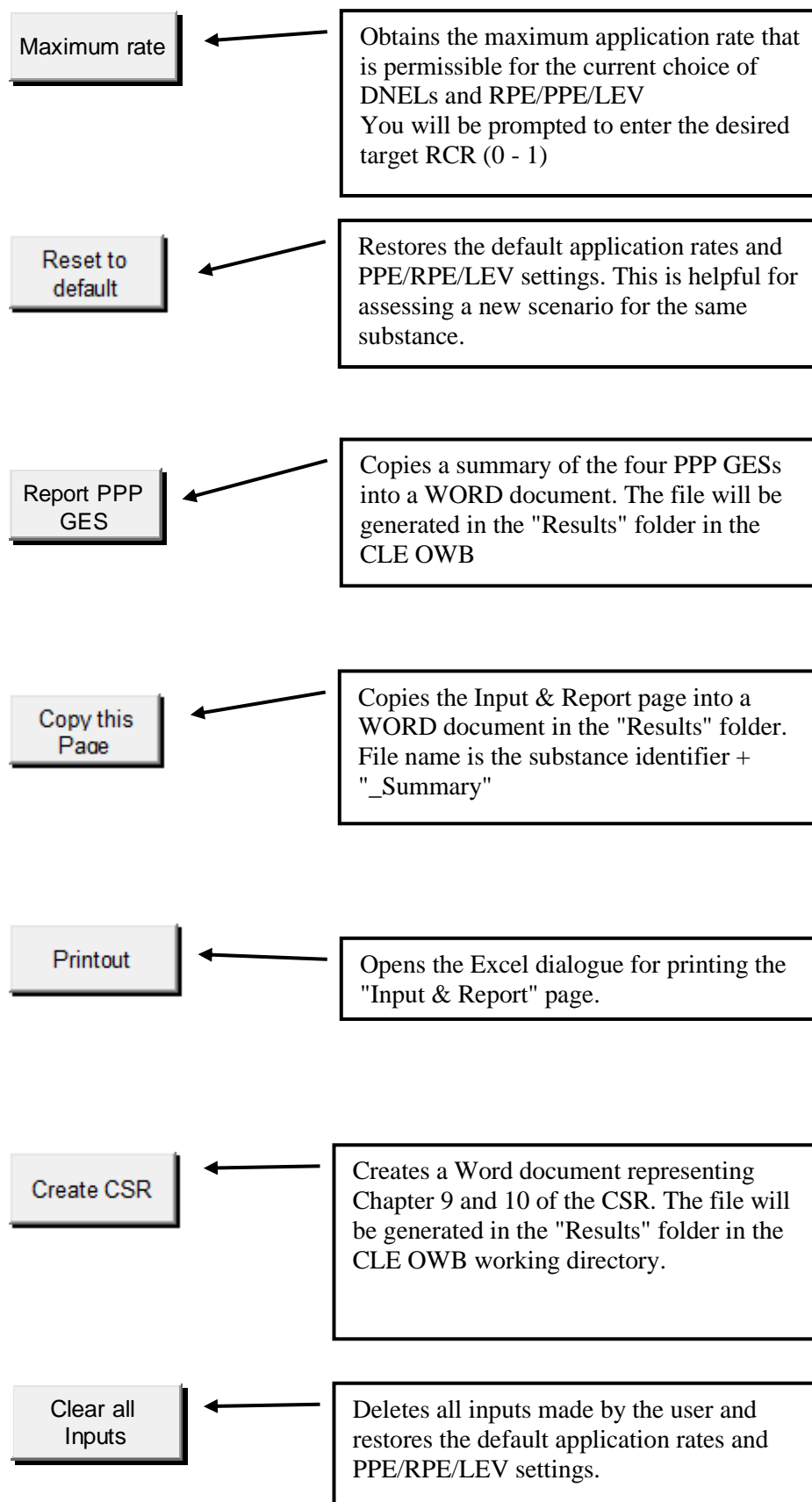
### 2.4.3 Results

The "Results" table will be populated as the necessary hazard and scenario information is entered. The table summarises all input parameters and the resulting exposure estimates.

Results		
<b>Inhalation exposure [mg/m<sup>3</sup>]</b>		
Mixing / loading (PROC 8a)	0.056	0.0050
Application (PROC 8b, 11 or 8a)	0.014	0.350
RCR inhal	<b>0.070</b>	<b>0.355</b>
<b>Dermal exposure [mg/kg bw/day]</b>		
Mixing / loading (PROC 8a)	0.0069	2.93
Application (PROC 8b, 11 or 8a)	1.31	0.577
RCR dermal	<b>0.661</b>	<b>1.75</b>
<b>Combined routes</b>		
RCR total	<b>0.731</b>	<b>2.11</b>

RCRs greater than 1.0 will be highlighted by a red cell

### 2.4.4 Macro functions within the OWB tool



### 2.4.5 Working with the CSR file

The CSR Chapters 9 and 10 generated by CLE OWB's "Create CSR" function will be stored in the **"Results" folder that must be present** in the tool's working directory.

The user-generated file will bear the name entered as identifier followed by the suffix “\_CSR-9-10”. **Do not edit any of the files in the "Templates" folder.**

If both an environmental and a human health risk assessment are needed for the co-formulant, it is imperative that the OWB tool is run first before editing the environmental part. The environmental sections can be completed by copying the respective output tables generated by LET and pasting them into the CSR document.

The resulting CSR file can be pasted into the respective sections of an existing CSR. The template and the CSR Chapters 9 and 10 are designed to be compatible with a CSR document generated with the CSR Generator tool implemented in IUCLID.

The CSR generated by IUCLID **must be converted from .rtf to .docx format** (saved as MS Word 2003 or higher) **before the Chapters 9 and 10** generated by the OWB tool **can be pasted** into the CSR file generated by IUCLID or in Chesar.

The **conclusion on risk characterisation** must be added at the **end of each contributing scenario**. The conclusion must be phrased according to the outcome of the risk characterisation:

#### **Environment**

##### **Conclusion on risk characterisation:**

<< Insert here the conclusions on risk characterisation for environment (Table X). >>

*The RCRs for the environmental compartments are all <1 and indicate adequate control of risks for the environment under the conditions of use.*

*or*

*The RCR for the <name of compartment> are >1 and thus further refinement is needed for this exposure scenario.*

#### **Workers**

##### **Conclusion on risk characterisation:**

<< Insert here the conclusions on risk characterisation for PROCnn worst case RCR (Table Y). >>

*The RCRs are all <1 and indicate that the human health risk for workers is adequately controlled under the conditions of use.*

*or*

*The RCR for <name of activity> exceeds 1 and indicates that further refinement of use rates and/or personal protective equipment is needed.*

## 2.4.6 Extracting scenarios for risk communication (eSDS)

Your Excel workbook contains four tabs named “PPP GES 1” through “PPP GES 4” (see screenshot below). Each tab contains a summary of all contributing scenarios within a given exposure scenario. The reasonable worst-case combination of contributing scenarios is documented at the bottom of the worksheet.

You can copy and paste the summary into an eSDS or similar documents to facilitate risk communication through the supply chain.

Combined exposures within Worker population									
Exposures estimates calculated for worst-case "sentinel" value from each correlated task. The worst-case from tractor or hand-held spraying is carried forward as a conservative value for risk assessment.									
Contributing Scenarios	Use rate		Dermal exposure [mg/kg bw/day]	Inhalation Exposure [mg/m <sup>3</sup> ]	PPE	RPE	Dermal RCR	Inhalation RCR	Total RCR
	[kg/ha]	[kg/d]							
<b>Tractor-mounted boom spraying</b>									
PROC 8a: Mixing & loading WP formulation	1.00	50.00	0.867	0.6956	gloves	no RPE	0.867	0.6956	1.563
PROC 11: Tractor-mounted boom spraying			0.125	0.0007	no PPE	no RPE	0.125	0.0007	0.126
<b>PROC 8a+11</b>			<b>0.993</b>	<b>0.696</b>			<b>0.993</b>	<b>0.696</b>	<b>1.689</b>
<b>Tractor-mounted air-blast spraying</b>									
PROC 8a: Mixing & loading WP formulation	1.00	10.00	0.225	0.4308	gloves	no RPE	0.225	0.4308	0.656
PROC 11: Tractor-mounted air-blast spraying			0.536	0.0234	no PPE	no RPE	0.536	0.0234	0.560
<b>PROC 8a+11</b>			<b>0.762</b>	<b>0.454</b>			<b>0.762</b>	<b>0.454</b>	<b>1.216</b>
<b>Hand-held spraying</b>									
PROC 8a: Mixing & loading WP formulation into hand-held sprayer	1.00	4.00	0.106	0.0017	gloves	FP1, P1 and similar	0.106	0.0017	0.108
PROC 11: Hand-held spraying, indoors (greenhouse)			0.465	0.0017	no PPE	FP1, P1 and similar	0.465	0.0017	0.466
<b>PROC 8a+11</b>			<b>0.571</b>	<b>0.003</b>			<b>0.571</b>	<b>0.003</b>	<b>0.574</b>



## 2.5 Model Information summary

### 2.5.1 Introduction

#### Assessment of agrochemical uses

CropLife Europe (CLE, formerly European Crop Protection Association, ECPA) has developed four plant protection product Generic Exposure Scenarios (PPP GES) for assessing human and environmental exposure to non-active substances (co-formulants) resulting from their use in plant protection products (PPP). The GES have been built by an expert group using exposure models that are established in the EU and US for assessing human and environmental exposure to PPP (Dobe et al., 2017). The models have been adapted to suit the requirements of REACH, e.g., the need for calculation of a route-specific external exposure rather than a systemic exposure, and the application of the REACH use descriptor system.

The following application types of PPP by workers and consumers are covered by PPP GES (see Section 1):

- PPP GES 1: Use as a co-formulant in plant protection products, spray applications by professionals
- PPP GES 2: Use as a co-formulant in plant protection products, seed and granular applications by professionals

- PPP GES 3: Use as a co-formulant in plant protection products, spray applications by consumers
- PPP GES 4: Use as a co-formulant in plant protection products, seed and granular applications by consumers

The non-dietary human exposure scenarios associated with each GES are intended to integrate with the OWB tool, incorporating exposure models which are well-established for the safety assessment of PPP in the EU. Within a given contributing scenario (e.g., PROC) described by a GES, there may be several sub-activities described by the standard PPP models (e.g., loading liquids, powders, or granules into tractor-mounted or hand-held equipment). The largest exposure value calculated for one of these sub-activities is taken as a representative (“sentinel”) value for the overall contributing scenario. To maintain transparency a summary of all the considered sub-activities and their resulting estimated human exposures is presented as a table within the contributing scenario. However, only the worst-case exposure value is selected and carried forward for risk characterisation.

In accordance with the most recent EFSA guidance on human exposure, the following general parameters for exposure assessment are used (EFSA, 2022):

- Body weight, adults: 60 kg
- Respiratory volume, worker: 10 m<sup>3</sup>/ 8 h
- Respiratory volume, general population, adults: 3.18 m<sup>3</sup>/ h

The most significant exposure determinant in standard PPP exposure models is the application rate (normally in kg/ha), which can be directly related to the potential exposure. To minimise “artificial” restrictions on co-formulant uses, the standard PPP exposure models were adapted for use under REACH to report the maximum application rate for a desired target RCR. For example, if a target RCR of 0.1 was specified, the maximum application rate which delivers this RCR is calculated iteratively.

The individual models implemented in OWB are explained in the following sub-sections.

## ***2.5.2 PPP GES 1: Use as a co-formulant in plant protection products, spray applications by professionals***

### *2.5.2.1 Description of the activities and technical processes covered in the exposure scenario:*

This exposure scenario covers the professional use of a co-formulant in PPP, applied as a spray. This scenario includes both indoor and outdoor use.

This generic exposure scenario covers the following tasks:

- the transfer (and inherent dilution and mixing) of solid and liquid PPP which occurs during loading of tractor-mounted/trailed boom sprayers, loading of tractor-mounted/trailed broadcast air-assisted sprayers, and loading of hand-held spray equipment;
- the spray application of PPP using tractor-mounted/trailed boom sprayers, tractor-mounted/trailed broadcast air-assisted sprayers, and hand-held spray equipment for high-level targets;
- the indirect exposure of workers on field re-entry and of bystanders.

Several established models are available for the assessment of operator exposure to (active) substances in PPP. These are implemented in an EFSA online calculator that is used for estimation of non-dietary exposure<sup>1</sup>, based on the current “Guidance on the assessment of exposure of operators, workers, residents and bystanders in risk assessment of plant protection products” (EFSA, 2022).

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<sup>1</sup> Available at <https://r4eu.efsa.europa.eu/app/opex> (accessed 01 Dec 2023)

This EFSA calculator estimates 75<sup>th</sup> and 95<sup>th</sup> percentiles of exposure of operators, workers, bystanders, and residents. Tractor-mounted/trailed and hand-held spray or granular applications are covered. Indoor and outdoor scenarios can be considered.

#### 2.5.2.2 *Worker contributing scenario 1: "Mixing and loading of plant protection products into delivery equipment" [PROC 8a]*

The contributing scenario covers the transfer (and inherent diluting and mixing) of solid and liquid PPP which occurs during loading of tractor-mounted/trailed boom sprayers, loading of tractor-mounted/trailed broadcast air-assisted sprayers, and loading of hand-held spray equipment.

The OWB calculates exposures varying all the variable exposure determinants within the respective models associated with loading of solid and liquid PPP into delivery equipment. The worst-case "sentinel" value for these sub-activities is carried forward as the generic conservative PROC 8a exposure value for the contributing scenario for risk assessment.

Since the EFSA model covers both inhalation and dermal exposure estimates it is used for the assessment. The studies and data underlying the EFSA model mostly reflect exposure to spray mist, as the active substances covered by the data are mostly non-volatile substances with a low vapour pressure under environmental conditions. Volatile co-formulants have to be assessed with some care. Nevertheless, more recent data (Fraunhofer 2018) suggest that models based on exposure to spray mists can be useful for a screening exposure assessment for substances with vapour pressures in the range from 10-100 Pa, but care must be taken with additional uncertainties.

Three distinct formulation types have been considered in the OWB tool: liquids, granules, and powders. Handling of powders potentially results in the highest exposure during mixing and loading (PROC 8a).

The mixing and loading of the PPP (as a liquid, granule, or powder) considered in the EFSA model can be translated into the REACH process category PROC 8a.

Unless specified, the EFSA model considers a layer of normal work wear covering arms, body, and legs. In the OWB tool, gloves are assumed to be worn by default during any mixing and loading activities, in accordance with good working practices promoted by CLE.

Two distinct tractor-mounted application types are considered: tractor-mounted ground-boom spraying onto low crops and air-blast spraying, e.g., onto trees. Ground-boom spraying has a higher daily work rate than air-blast spraying (assumed 50 ha and 10 ha, respectively). As a result, more substance is handled for ground-boom spraying which therefore usually constitutes the worst case for the mixing and loading contributing scenario, unless gloves are worn during mixing and loading. In this case, air-blast spraying may become the worst-case for the contributing scenario covering the loading of tractor-mounted equipment.

For outdoor hand-held spraying, a daily work rate of either 4 or 1 ha is assumed in the model, for spray lances attached to a large tank or a knapsack, respectively. For all indoor applications, 1 ha is the default daily work rate. The corresponding amount of substance handled per day is considered for assessing exposure resulting from mixing and loading.

The amount of co-formulant handled per day depends on the application rate (kg substance applied per ha) as well as the size of the application area (ha per day). However, the amount of co-formulant handled per day is not a variable in the exposure calculations for knapsack sprayers; instead, a fixed exposure ( $\mu\text{g}$  substance per day) is assumed for the mixing and loading contributing scenario. As a result, an unacceptable risk for knapsack sprayers cannot be mitigated by a reduction of the allowable amount of co-formulant handled per day. Thus, the data for knapsack sprayers cannot be used to identify the amount of a co-formulant that can be safely handled per day. The lance-on-tank scenario with its larger default application area (4 ha/day) is scalable by the amount of co-formulant used on a daily basis and therefore is used as worst-case contributing scenario for mixing and loading covering all types of hand-held applications. OWB will determine the worst case for the given constellation by calculating the total RCR for the combined routes. Only the worst-case result will be carried forward to risk assessment.

The transfer of solid and liquid PPP which occurs during loading of tractor-mounted/trailed boom sprayers, loading of tractor-mounted/trailed broadcast air-assisted sprayers, and loading of hand-held spray equipment is considered for all the variable exposure determinants within the EFSA model.

The worst-case “sentinel” value (typically a wettable powder (WP) formulation type) for these sub-activities is carried forward for risk characterisation as the generic conservative PROC 8a value for this contributing scenario.

**Table 1:** Typical CLE OWB output table (PROC8a) showing exposure estimates for all variable exposure determinants within the EFSA model for mixing and loading: three possible tasks, each of which estimates an exposure for liquids, powders, granules. The worst-case "sentinel" value is highlighted in bold.

Type of equipment and conditions	Model	Formulation type	Dermal exposure [mg/kg bw/day]	Inhalation Exposure [mg/m <sup>3</sup> ]	Total RCR
Mixing and loading tractor mounted/ trailed boom sprayer	EFSA	Liquid	0.019	0.0008	0.020
		Powder (WP)	0.299	0.5714	<b>0.870</b>
		Granule (WG)	0.010	0.0061	0.016
Mixing and loading tractor mounted/ trailed broadcast air-assisted sprayer	EFSA	Liquid	0.005	0.0004	0.006
		Powder (WP)	0.113	0.3100	0.423
		Granule (WG)	0.036	0.0033	0.040
Mixing and loading hand-held sprayer, outdoors	EFSA	Liquid	0.006	0.0005	0.007
		Powder (WP)	0.125	0.3607	0.486
		Granule (WG)	0.004	0.0039	0.007
Mixing and loading hand-held sprayer, indoors	EFSA	Liquid	0.002	0.0003	0.003
		Powder (WP)	0.054	0.2130	0.267
		Granule (WG)	0.001	0.0023	0.004

### 2.5.2.3 Worker contributing scenario 2: "Delivery and dispersion of plant protection products" [PROC 11]

The contributing scenario covers the spray application of PPP using tractor-mounted/trailed boom sprayers, tractor-mounted/trailed broadcast air-assisted sprayers, and hand-held spray equipment for high-level targets, as well as the indirect exposure of workers on field re-entry and bystanders.

The OWB calculates exposures varying all the variable exposure determinants within the respective models associated with the spraying of PPP. The worst-case “sentinel” value for these sub-activities is carried forward as the generic conservative PROC 11 exposure value for the contributing scenario for risk assessment. While not explicitly considered in industrial exposure assessments, worker re-entry and indirect exposure of bystanders are included as they form part of the typical risk assessment paradigm used in agrochemical exposure assessments.

If required in a refinement, this contributing scenario can be split into separate PROC 11 contributing scenarios for tractor-mounted and for hand-held spraying. However, to keep the exposure scenarios as short as possible, the initial assumption is that the two application types can be combined, potentially with differing PPE requirements.

Exposure from the spray application of PPP is independent of the initial formulation types since dilution/dispersion into water has usually occurred. The spray application of the liquid, diluted PPP considered in the EFSA model can be translated into the REACH process category PROC 11.

Within PROC 11, the model considers both mechanical spraying (tractor-mounted) as well as hand-held spraying (spray gun, knapsack). Unless explicitly specified, the EFSA model considers a layer of normal work wear covering arms, body, and legs.

Two distinct tractor-mounted application types are considered: tractor-mounted ground-boom spraying onto low crops and air-blast spraying on high-standing crops, e.g., onto trees. Ground-boom spraying has a much higher daily work rate than air-blast spraying (assumed 50 ha and 10 ha, respectively). As a result, more substance is handled for ground-boom spraying. On the other hand, air-blast spraying is likely to produce considerably more aerosols than ground-boom spraying. Thus, the overall exposure potential for air-blast spraying is higher in this contributing scenario for spray application of PPP.

For vehicle-mounted applications, both downward spraying (representing ground-boom spraying) and upward spraying (air-blast application in orchards or other high-growing cultures) were adopted for OWB. The EFSA model has different parameter sets for various body parts exposed via the dermal route: body, hands, and head. Values for unprotected and protected body and hands are available. “Unprotected body” is equivalent to an operator wearing no clothes at all, which is not a realistic scenario and therefore was not adopted for the OWB tool. “Protected body” refers to an operator donning work wear with arms, trunk and legs covered, whereas “protected hands” means that suitable chemical-resistant gloves are worn.

For hand-held spraying, both upward and downward spraying directions are considered in OWB. While upward spraying has a higher potential for inhalation exposure, downward spraying entails a much higher potential dermal exposure. Which direction is worst case will depend on the relative magnitude of inhalation and dermal DNELs. OWB will determine the worst case for the given constellation by calculating the total RCR for the combined routes. Only the worst-case result will be carried forward to risk assessment. The model assumes a daily work rate of 4 or 1 ha for manual spraying with lances connected to a large tank or a knapsack tank, respectively. Special options of the EFSA model like use of spray trolleys, dense cultures, wearing of rain suits, etc., are not implemented in OWB to maintain its character as a screening-level tool.

**Table 2:** Typical CLE OWB output table (PROC11) showing exposure estimates for all variable exposure determinants: four possible tasks within the EFSA model for spraying, and two additional models. The worst-case "sentinel" value is highlighted in bold.

Type of equipment and conditions	Model	Formulation type	Dermal exposure [mg/kg bw/day]	Inhalation Exposure [mg/m <sup>3</sup> ]	Total RCR
Tractor mounted/ trailed boom spraying	EFSA	Liquid	0.029	0.0004	0.030
Tractor mounted/ trailed broadcast air-assisted spraying			0.148	0.0152	0.163
Hand-held spraying, downwards, outdoors			0.408	0.0061	0.414
Hand-held spraying, upwards, indoors			0.449	0.0430	<b>0.492</b>
Worker re-entry (indirect exposure)			0.4911	0.0504	0.542
Professional Bystander (indirect exposure)			0.4412	0.1136	0.555



#### 2.5.2.4 Consideration of Worker Re-entry

While not explicitly considered in industrial exposure assessments, worker exposure resulting from re-entry of areas treated with a PPP is included here as it forms part of the typical risk assessment paradigm used for agrochemicals. Because exposure arising from worker re-entry is not a formal ‘use’ of the substance, it is included within the spray scenario, rather than as a separate contributing scenario (see GES development in Dobe et al., 2017).

Workers re-entering treated cultures are potentially exposed to dislodgeable foliar residues (DFR). The only significant potential for worker exposure following re-entry will be contamination via the skin. Inhalation exposure is considered to be negligible. If a co-formulant is volatile (at this time scale volatility is defined by a vapour pressure  $\geq 0.1$  Pa), then the DFR is zero 24 hours after application due to complete evaporation of the substance.

For non-volatile co-formulants, the default initial DFR of  $3 \mu\text{g}/\text{cm}^2$  per kg substance/ha is adopted from the EFSA model. External dermal exposure of workers (re-)entering treated cultures ( $E_{D, \text{worker}}$ ) is calculated using the following equation:

$$E_{D, \text{worker}} [\text{mg}/\text{kg bw}/\text{day}] = TC \times ET \times DFR_{\text{initial}} \times AR / 1000 / BW \quad \text{Equation 1}$$

Where:

- *TC*: transfer coefficient [ $\text{cm}^2/\text{h}$ ]
- *ET*: exposure time [ $\text{h}/\text{day}$ ]
- *DFR<sub>initial</sub>*: dislodgeable foliar residue [ $\mu\text{g}/(\text{cm}^2 \times \text{kg}/\text{ha})$ ]
- *AR*: application rate [ $\text{kg}/\text{ha}$ ]
- *BW*: body weight [ $\text{kg}$ ]

It is considered that the evaluation of exposure for a re-entry situation directly after application (spray deposit has dried) and using high end default values for each parameter results in a very conservative risk assessment.

#### Considerations on Transfer Coefficients:

The EFSA model has transfer coefficients (TCs) for twenty different crop types with matching exposure times. These options have been made available in OWB and can be used for a crop-specific assessment. However, registrants of substances used as a co-formulant will often lack the knowledge of the crop types that are treated with PPP containing the specific co-formulant. Per default, OWB will use a 75<sup>th</sup> percentile TC value that is applicable for the “all crops” category given in the EFSA guidance (EFSA, 2022). This general category applies to a variety of cultures like cereals, grassland and lawns, hops, oilseeds, root and tuber vegetables, and sugar beets. A daily exposure duration (ET) of 8 hours is assumed. Workers are expected to wear normal work clothing with arms, legs, and trunk covered ( $TC=1400 \text{ cm}^2/\text{h}$ ). TCs for gloved hands are not available for the general crop category. As a surrogate the respective TC value of  $1250 \text{ cm}^2/\text{h}$  is adopted from vegetables (Table 3).

Where a risk assessment for local dermal effects is required, dermal exposure is normalised to the surface of the palms of both hands, with an assumed surface area of  $420 \text{ cm}^2$ . This is a conservative approach since it assumes that the external dermal dose completely adheres to the hands, whereas in reality, the dose is distributed over the entire (clothed) body surface.

**Table 3:** Exposure parameters for the assessment of exposure of workers during re-entry.

Variable	Value	Unit	Explanation
<i>TC</i>	1400	cm <sup>2</sup> /h	Transfer coefficient, normal work clothing, 75 <sup>th</sup> percentile
	1250		Transfer coefficient, normal work clothing plus gloves, 75 <sup>th</sup> percentile
<i>ET</i>	8	h/day	Daily exposure duration
<i>DFR<sub>initial</sub></i>	3	µg/(cm <sup>2</sup> × kg/ha)	Dislodgeable foliar residue, normalised to application rate
<i>BW</i>	60	kg	Body weight, adults

### Considerations on Worker Inhalation Exposure:

Inhalation task-specific factors (TSF) have been estimated for a small set of exposure data for harvesting and re-entry in ornamental greenhouses (van Hemmen et al., 2002). The current EFSA guideline (2022) proposes that these TSFs are adopted for all greenhouse crops in a screening assessment, where exposure is estimated as follows:

$$PIE = AR \times TSF \times ET \quad \text{Equation 2}$$

where:

- *PIE* = potential inhalation exposure (mg a.s./h inhaled)
- *AR* = application rate (kg a.s./ha)
- *TSF* = task-specific factor [(mg a.s./h)/(kg a.s./ha)]
- *ET* = exposure time (8 h/day)

For cutting, bundling and other harvest activities, a TSF of 0.1 (mg a.s./h) / (kg a.s./ha) should be applied. For re-entry activities like inspection, general maintenance, sorting, or watering, a TSF of 0.01 (mg a.s./h) / (kg a.s./ha) is proposed. The worst-case TSF of 0.1 (mg a.s./h) / (kg a.s./ha) is used in OWB for worker re-entry inhalation exposure assessment.

In the CLE OWB, vapour pressure and molecular weight of the co-formulant can be entered by the user for calculation of the saturated vapour concentration (SVC) according to EFSA (2022):

$$SVC = 0.41 \times MW \times VP \quad \text{Equation 3}$$

where:

- *SVC* = saturated vapour concentration (mg/m<sup>3</sup>)
- *MW* = molecular weight (g/mol)
- *VP* = vapour pressure (Pa)

The SVC sets an upper physical limit for vapour exposure in greenhouses. In cases where the PIE estimate based on the TF exceeds the estimate based on the SVC, the potential inhalation exposure is calculated as follows:

$$PIE = SVC \times IR$$

Equation 4

where:

– *IR* = inhalation rate (10 m<sup>3</sup>/day)

#### 2.5.2.5 Consideration of Exposure of Bystanders

While not explicitly considered in most industrial exposure assessments, exposure of bystanders to spray drift and deposit is included here as it forms part of the typical risk assessment paradigm used for agrochemicals. Exposure of bystanders results from the use of the substance, but it is not a "use" itself, and hence is included within the spray scenario, rather than as a separate contributing scenario (see GES development in Dobe et al., 2017). The use descriptor system is therefore not relevant in this case.

The EFSA model predicts bystander exposure for members of the general public, whose presence in the vicinity of a treated field is incidental and not related to the application of the PPP but who may experience short-term exposure due to their presence. In the EFSA model, the predicted short-term exposure can be compared to a threshold value for an acutely toxic substance. Where members of the general public are anticipated to experience irregular and short-term bystander exposure to spray drift containing an acutely very toxic substance, an acute exposure estimate is required for comparison with a general population short-term DNEL. However, it is anticipated that agricultural workers carrying out other activities in the area of PPP application have the potential to be exposed regularly to spray drift as bystanders, resulting in repeated or longer-term exposure to co-formulants. As a result, in the spray exposure scenario implemented in the OWB tool, long-term exposure to spray drift and vapour is predicted for professional users by applying the methodology of the EFSA guidance for comparison with a long-term DNEL. In the following, the term "bystander" refers to workers carrying out activities in the area of PPP application but who are not operators.

The worst-case drift rate that can result in bystander exposure is anticipated for upward spraying in orchards using broadcast air assisted sprayers. The 75<sup>th</sup> percentile parameters provided in the EFSA guidance are used (Table 4). Light clothing (shoes, shorts, T-shirt) is assumed for workers considered as bystanders. The potential exposure of bystanders is reduced by 18% by light clothing. The water application rate (L/ha) is a variable in the EFSA model but is fixed to 100 L water/ha in OWB as a reasonable worst case to limit the number of necessary input parameters.

The dermal exposure of bystanders is calculated with the following equation:

$$E_{D, \text{drift}} \text{ (mg/kg bw/day)} = DE_{\text{drift}} \times (1-LCAF) \times C_{\text{dil}} \times 1000 / BW$$

Equation 5

Where:

–  $DE_{\text{drift}}$  = dermal exposure to spray drift (mL/person)

–  $LCAF$  = light closing adjustment factor (18%)

–  $C_{\text{dil}}$  = concentration of co-formulant in spray dilution (kg/L)

–  $BW$  = body weight (kg)

Drift data are adopted from the EFSA guidance (EFSA 2022). A distance of 10 m aiming in upward direction from the spray equipment is assumed. Calculations of bystander exposure are performed only for this worst-case scenario. In addition to spray drift, there may also be vapour drift of volatile substances. In accordance with current practices for the assessment of bystander exposure to active ingredients of PPP, the vapour drift exposures are added to the spray drift exposure depending on the

vapour pressure of the co-formulant. Default parameter values used in the calculation of inhalation exposure are shown in Table 4.

**Table 4:** Exposure parameters for the assessment of exposure of bystanders.

Variable	Value	Unit	Explanation
$DE_{\text{drift}}$	3.68	mL/person	dermal exposure of adult to spray drift, upward spraying, 75 <sup>th</sup> percentile
$IE_{\text{drift}}$	0.002	mL/person	inhalation exposure of adult to spray drift, upward, 75 <sup>th</sup> percentile
$LCAF$	18%	%	Light clothing adjustment factor
$BW$	60	kg	Body weight, adult
$IR$	0.053	m <sup>3</sup> /h/kg bw	Inhalation rate, adult
$C_{\text{vapour}}$	0.000	mg/m <sup>3</sup>	Concentration in air of substance with negligible volatility, i.e., $VP^* < 0.00001$ Pa
	0.001	mg/m <sup>3</sup>	Concentration in air of substance with low volatility, i.e., $0.00001 \text{ Pa} < VP < 0.005 \text{ Pa}$
	0.015	mg/m <sup>3</sup>	Concentration in air of substance with medium or high volatility, i.e., $VP \geq 0.005 \text{ Pa}$

<sup>a</sup> VP: vapour pressure of the co-formulant at 25 °C

Inhalation exposure of bystanders to spray drift ( $E_{I, \text{drift}}$ ) is calculated by the following equation:

$$E_{I, \text{drift}} \text{ (mg/m}^3\text{)} = IE_{\text{drift}} \times C_{\text{dil}} \times 1000 / BW / IR \quad \text{Equation 6}$$

Where:

- $IE_{\text{drift}}$  = inhalation exposure to spray drift (mL/person)
- $C_{\text{dil}}$  = concentration of co-formulant in spray dilution (kg/L)
- $BW$  = body weight (kg)
- $IR$  = inhalation rate (m<sup>3</sup>/day/kg bw)

#### 2.5.2.6 Consideration of residential exposure

The EFSA guidance describes a procedure for the estimation of “residential exposure” which may arise from crop protection uses. The models for the assessment of residential exposure have been included in the OWB in the “Residential” tab, in accordance with the EFSA guidance, based on reasonable worst-case input parameter values. The “Residential” tab can be used for an ad-hoc assessment of residential exposure, should this be required. On a case-by-case basis this may be necessary for a limited number of substances, which can exhibit significant acute toxicity, and this is coupled with physical-chemical properties potentially leading to high peak exposure by a relevant route (e.g., very high vapour

pressures). The exposure occurring via the assessed pathways should be interpreted as short-term exposure in the context of REACH risk assessments, and thus compared to short-term systemic DNELs. It should be noted that the DNELs for the general public required in the OWB “Input & Report” tab are for long-term systemic effects, and these values should not be used for the assessment of potential risks resulting from residential exposure calculated according to the EFSA guidance. DNELs established for short-term, systemic effects occurring via the inhalation, dermal or oral route can be entered in the “Residential” tab, if an assessment of acute exposure of residents is performed. It should also be noted that in the REACH context long-term exposure of the general public to substances used as a co-formulant in plant protection products is considered to be assessed as indirect exposure of man via the environment as part of the environmental exposure assessment (see the LET for details on approach), rather than as part of the worker exposure assessment.

### 2.5.2.7 Exposure estimation for combined contributing scenarios

The mixing and loading, as well as spray application of PPP, are correlated contributing scenarios because they are usually carried out in conjunction by the same workers. The table below reports the relevant combined worst-case exposures from PROCs 8a and 11.

Because of the correlation, these combined RCRs are used in the algorithm to maximise the application rate of a co-formulant for a given a target RCR.

**Table 5:** Typical CLE OWB output table showing exposure estimates for correlated tasks across contributing scenarios in GES1.

Contributing Scenarios	Use rate		Dermal exposure [mg/kg bw/day]	Inhalation Exposure [mg/m <sup>3</sup> ]	PPE	RPE	Dermal RCR	Inhalation RCR	Total RCR
	[kg/ha]	[kg/d]							
<b>Tractor-mounted boom spraying</b>									
PROC 8a: Mixing & loading WP formulation	0.24	11.77	0.299	0.5714	gloves	no RPE	0.299	0.5714	0.870
PROC 11: Tractor-mounted boom spraying			0.029	0.0004	no PPE	no RPE	0.029	0.0004	0.030
<b>PROC 8a+11</b>			<b>0.328</b>	<b>0.572</b>				<b>0.328</b>	<b>0.572</b>
<b>Tractor-mounted air-blast spraying</b>									
PROC 8a: Mixing & loading WP formulation	0.24	2.35	0.113	0.3100	gloves	no RPE	0.113	0.3100	0.423
PROC 11: Tractor-mounted air-blast spraying			0.148	0.0152	no PPE	no RPE	0.148	0.0152	0.163
<b>PROC 8a+11</b>			<b>0.261</b>	<b>0.325</b>				<b>0.261</b>	<b>0.325</b>
<b>Hand-held spraying, indoors</b>									
PROC 8a: Mixing & loading WP formulation into hand-held sprayer	0.88	3.51	0.054	0.2130	gloves	no RPE	0.054	0.2130	0.267
PROC 11: Hand-held spraying, indoors (greenhouse)			0.449	0.0430	no PPE	no RPE	0.449	0.0430	0.492
<b>PROC 8a+11</b>			<b>0.503</b>	<b>0.256</b>				<b>0.503</b>	<b>0.256</b>
<b>Hand-held spraying, outdoors</b>									
PROC 8a: Mixing & loading liquid formulation into hand-held sprayer	0.88	3.51	0.125	0.3607	gloves	no RPE	0.125	0.3607	0.486
PROC 11: Hand-held spraying, outdoors			0.408	0.0061	gloves	no RPE	0.408	0.0061	0.414
<b>PROC 8a+11</b>			<b>0.533</b>	<b>0.367</b>				<b>0.533</b>	<b>0.367</b>

## 2.5.3 PPP GES 2: Use as a co-formulant in plant protection products, seed and granular applications by professionals

### 2.5.3.1 Description of the activities and technical processes covered in the exposure scenario:

This exposure scenario covers the professional use of a co-formulant in PPP, applied in granular form or as treated seeds. This scenario includes both indoor and outdoor use.

This generic exposure scenario covers the following tasks:

- the transfer of treated seed and granular PPP which occurs during loading of tractor-mounted broadcast spreaders, and the loading of mechanical equipment with solid and liquid PPP for the treatment of seeds;
- the loading of manual belly-grinders and “push-type” spreaders;
- the transfer of treated seeds from a batch treater into bags;
- the delivery and dispersion of treated seeds and granular PPP from manual spreading (by hand), mechanical spreading (belly grinders and push-type rotary spreaders), and from tractor-mounted broadcast spreaders.

#### 2.5.3.2 Worker contributing scenario 1: "Mixing and loading of plant protection products into seed treatment or delivery equipment" [PROC 8a]

The contributing scenario covers the transfer of treated seed and granular PPP which occurs during loading of tractor-mounted broadcast spreader and the loading of manual belly-grinders and “push-type” spreaders.

The OWB calculates exposures varying all the variable exposure determinants within the respective models associated with loading of solid and liquid PPP into delivery equipment. The worst-case "sentinel" value for these sub-activities is carried forward as the generic conservative PROC 8a exposure value for the contributing scenario for risk assessment.

The activities covered by this scenario include the loading of treated seeds or granular PPP into delivery equipment. These tasks can be translated into the systematic use descriptor PROC 8a.

Exposure emerging from the loading of granular PPP or treated seeds into a hopper is assessed using the EFSA implementation of the US Environmental Protection Agency “The Pesticide Handler Exposure Database” (PHED, scenario Mixing/Loading Granules)<sup>2</sup> and the following equations:

$$E_{\text{dermal}} = AR \times A \times UE_{\text{route}} / BW \quad \text{Equation 7}$$

$$E_{\text{inh}} = AR \times A \times UE_{\text{route}} / RV \quad \text{Equation 8}$$

Where:

- $E_{\text{dermal}}$  = Dermal exposure, systemic (mg/kg bw)
- $E_{\text{inh}}$  = Inhalation exposure (mg/m<sup>3</sup>)
- $AR$  = Application rate (mg/ha)
- $A$  = Area (ha/day)
- $UE_{\text{route}}$  = Unit exposure for the relevant route and quantity handled (mg/kg)
- $BW$  = Body weight (kg)
- $RV$  = Respiratory volume (m<sup>3</sup>/day)

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<sup>2</sup> US Environmental Protection Agency - Office of Pesticide Programs: Occupational Pesticide Handler Unit Exposure Surrogate Reference Table, March 2012, available at <http://www.epa.gov/pesticides/science/handler-exposure-table.pdf> (accessed 8 Jun 2012)

The 75<sup>th</sup> percentile default values and assumptions given in Table 6 were adopted in OWB for assessing the loading of granular PPP or treated seeds (EFSA, 2022).

**Table 6:** Exposure parameters for the assessment of granular products and treated seeds.

Variable	Value	Comment
AR	20 kg/ha (or maximised)	Default application rate (or maximised to a specified RCR)
A	50 ha	Default area for tractor
UE <sub>body</sub>	0.016 mg/kg	Unit value per kg substance handled, light clothing
UE <sub>hand</sub>	0.0015 mg/kg	Unit value per kg substance handled, gloves
UE <sub>inhalation</sub>	0.021 mg/kg	Unit value per kg substance handled, no RPE
BW	60 kg	EFSA default
RV	10 m <sup>3</sup> /day	REACH worker default, light work

Exposure values are 75<sup>th</sup> percentiles of the exposure distribution, as given in the EFSA tool and calculated from original PHED data. Original PHED values initially include personal protective equipment. EFSA assumes a protection factor of 100 to estimate potential exposure of the unprotected skin (i.e., PHED values are multiplied by 100 to calculate the dermal exposure). OWB adopts this approach. The default in OWB is that the body of operators handling granules is covered (long-sleeve shirt, long pants, shoes plus socks) and gloves are worn during mixing and loading.

**Table 7:** CLE OWB output table (PROC8a) for GES2

Type of equipment and conditions	Model	Formulation type	PPE	RPE	Dermal exposure [mg/kg bw/day]	Inhalation Exposure [mg/m <sup>3</sup> ]	Total RCR
Mixing and loading granules/treated seeds	PHED	Solid (GR)	no PPE	no RPE	0.283	2.0810	2.364

#### 2.5.3.3 Worker contributing scenario 2: “Transfer of treated seeds from batch treater into bags” [PROC 8b]

The current version of the OWB tool does not contain models that can be used to assess seed treatment. The approach used in previous versions has been deprecated in favour of a separate tool for the assessment of seed treatment which is currently being developed outside of the REACH-IN project. Reintroduction will be considered when the dedicated models for seed treatment become public.

#### 2.5.3.4 Worker contributing scenario 3: “Delivery and dispersion of agrochemical plant protection products or treated seeds” [PROC 8a]

The contributing scenario covers the delivery and dispersion of treated seeds and granular PPP from manual spreading (by hand), mechanical spreading (belly grinders and push-type rotary spreaders), and from tractor-mounted broadcast spreaders.

The OWB calculates exposures varying all the variable exposure determinants within the respective models associated with exposure arising from dispersion of granular PPP or treated seeds. The worst-case “sentinel” value for these sub-activities is carried forward as the generic conservative PROC 8a value for the contributing scenario for risk assessment.

This contributing scenario is not relevant for substances used as solvents. It can be expected that solvents are generally volatile substances that evaporate already during the seed treatment process. Thus, the greatest fraction of the solvent is anticipated to be evaporated before treated seeds are dispersed. Similarly, only a negligible loading of a liquid in a granular PPP is possible while maintaining physical integrity.

Dispersion of granular PPP or pre-treated seeds can be conducted with tractor-mounted equipment or using hand-held equipment. In rare cases, granular formulations or treated seeds can also be applied directly by hand. EFSA reviewed the PHED data (US EPA, 2012) and implemented models for dispersion by hand or with tractor-mounted equipment in the EFSA model. These activities can be translated into the systematic use descriptor PROC 8a. Manual dispersion is assumed to apply to smaller areas not exceeding 200 m<sup>2</sup> according to PHED, but the area in the EFSA model was increased to 1 ha per day.

The parameters from the PHED models have been converted into metric units and rounded in the present EFSA guidance (EFSA, 2022). Use of working clothes (long-sleeve shirt, long pants, shoes plus socks) is assumed in the PHED unit exposure values. When gloves are assigned to a task, this is accounted for by using the PHED data for gloved hands. The default protection factor of gloves within the PHED model is 10. This default is used where measured data to account for the presence or absence of gloves are not available. An exception to this default is the EFSA approach of estimating potential skin exposure to granulated PPP by multiplying actual exposure values with an assumed protection factor of 100. This approach is adopted in OWB to maintain compatibility with the EFSA calculator. Nevertheless, the approach applied by EFSA will lead to an overprediction of actual operator exposure resulting from the handling of granular products and treated seeds.

The default area treated per day using tractor-mounted equipment is 50 ha and the corresponding treated area treated per day by manual dispersion is 1 ha.

Indoor dispersion of granules or treated seeds will be in greenhouses which have large volumes and good ventilation. Granular PPP and treated seeds do not contain volatile substances and exposure via inhalation is expected to be low compared to dermal exposure. The exposure during application of granular PPP or treated seeds by hand-held equipment is thus expected to be very similar between outdoor and indoor settings. The indoor dispersion of such materials is therefore also covered by this contributing scenario.

See the preceding equations (Equation 7 and Equation 8) for calculation of exposures from PHED. The 75<sup>th</sup> percentile default values shown in Table 8 were adopted in OWB in addition to those previously specified (EFSA, 2022).

**Table 8:** Default unit exposure values used to estimate operator exposure resulting from the handling of granules or treated seeds.



Scenario	Variable	Value	Comment
Applicator, Granules by Hand	$UE_{body}$	69 mg/kg substance	Unit value for covered body per kg handled, no PPE
	$UE_{hand}$	29 mg/kg substance	Unit value for hand per kg handled, gloves
	$UE_{inhalation}$	0.4677 mg/kg substance	Unit value per kg handled, no RPE
Applicator, Open Cab Solid Broadcast Spreader	$UE_{body}$	0.0047 mg/kg substance	Unit value for covered body per kg handled, no PPE
	$UE_{hand}$	0.0041 mg/kg substance	Unit value for hand per kg handled, gloves
	$UE_{inhalation}$	0.0012 mg/kg substance	Unit value per kg handled, no RPE
Spreading by hand	$A$	1 ha	Area treated by hand application
Mechanical, powered	$A$	50 ha	Area treated by tractor
Mechanical or manual spreading	$AR$	20 kg/ha (or maximised)	Default application rate (or maximized to a specified RCR)

**Table 9:** Typical CLE OWB output table (PROC8a) for GES2 showing exposure estimates for tasks associated with the application of solid, granular products.

Type of equipment and conditions	Model	Formulation type	PPE	RPE	Dermal exposure [mg/kg bw/day]	Inhalation Exposure [mg/m <sup>3</sup> ]	Total RCR
Applicator, Granules by Hand	PHED	Solid (GR)	Work wear + gloves	no RPE	0.871	0.029	0.900
Applicator, Open Cab Solid Broadcast Spreader			Work wear + gloves	no RPE	0.003	0.008	0.011

#### 2.5.3.5 Exposure estimation for combined contributing scenario worker exposure

The mixing and loading of granular PPP and treated seeds, as well as the dispersion of these products, are correlated tasks as they are usually carried out in conjunction by the same workers. Because of the correlation the combined RCRs are used in the calculation of the maximal safe application rate of a co-formulant for a given target RCR.

**Table 10:** Typical CLE OWB output table showing exposure estimates for correlated tasks across contributing scenarios in GES2.

Contributing Scenarios	Use rate		Dermal exposure [mg/kg bw/day]	Inhalation Exposure [mg/m <sup>3</sup> ]	Dermal RCR	Inhalation RCR	Total RCR
	[kg/ha]	[kg/d]					
<b>Dispersion of granules or treated seeds, tractor</b>							
PROC 8a: Mixing and loading granules (including treated seeds)	<b>0.628</b>	<b>31.4</b>	0.009	0.065	0.009	0.065	0.074
PROC 8a: Applicator, open cab solid broadcast spreader			0.003	0.008	0.003	0.008	0.011
<b>PROC 8a+8a</b>			<b>0.011</b>	<b>0.074</b>	<b>0.011</b>	<b>0.074</b>	<b>0.085</b>
<b>Dispersion of granules or treated seeds, manual</b>							
PROC 8a: Spreading of granules or treated seeds by hand	<b>0.628</b>	<b>0.628</b>	<b>0.871</b>	<b>0.029</b>	<b>0.871</b>	<b>0.029</b>	<b>0.900</b>

## 2.5.4 PPP GES 3: Use as a co-formulant in plant protection products, spray applications by consumers

### 2.5.4.1 Description of the activities and technical processes covered in the exposure scenario:

This exposure scenario covers the consumer use of a co-formulant in PPP, applied as a spray. This scenario includes both indoor and outdoor use.

This generic exposure scenario covers the following tasks:

- the transfer (and inherent diluting and mixing) of solid and liquid PPP which occurs during loading of hand-held spray equipment;
- the spray application of PPP using hand-held spray equipment for high-level targets.

### 2.5.4.2 Consumer contributing scenario 1: "Spray application of agrochemical plant protection products"

The consumer use of PPP (home and garden) is infrequent and on a much smaller scale (200 m<sup>2</sup>/day) than professional use (1 to 50 ha/day). It cannot be anticipated that consumers wear PPE during the application of PPP. The EFSA model does not contain data for daily application amounts lower than 1.5 kg substance/day. For an area of 0.02 ha that is treated with a knapsack sprayer, this applied amount is equivalent to an application rate of 75 kg substance per ha, an application rate clearly exaggerating realistic worst-case figures (about 1 kg/ha) for co-formulants. However, the standard EFSA model algorithms do not allow scaling down to smaller, more realistic application rates. To extend the EFSA model to amateur uses, linear scaling of exposure estimates in relation to any application rate has been allowed within OWB.

The consumer use of PPP predominantly results in dermal and inhalation exposure. Predicted dermal exposures for volatile co-formulants can be expected to be worst-case because volatilisation from spray mist before deposition (Delmaar and Bremmer, 2009) and subsequent volatilisation from the skin is not accounted for. Similar to what has been discussed in section 2.5.2.2, the studies and data underlying the EFSA model mostly reflect exposure to spray mist, and volatile co-formulants have to be assessed with some care. Nevertheless, more recent data (Fraunhofer 2018) suggest that models based on exposure to spray mists can be useful for a screening exposure assessment for substances with vapour pressures in the range from 10-100 Pa, but care must be taken with additional uncertainties. Oral exposure can result

from inhalation of the non-respirable droplet fraction which is eventually swallowed. Since the model data for inhalation include the respirable as well as the non-respirable aerosol fraction, the risk assessment for the inhalation route inherently covers this route of oral exposure as well. Direct oral intake of PPP is considered to be accidental and beyond a reasonable worst-case scenario.

To account for the lack of training of amateur operators, the 95<sup>th</sup> percentile exposure parameters from the EFSA model database are used in OWB calculations. The amateur use implies that no protective clothes or gloves are worn. Thus, EFSA model parameters implying unprotected hands and body are used for mixing/loading and spraying by amateurs. Consumers are assumed to wear light clothes consisting of T-shirt, shorts, and shoes, but the moderate protection afforded by this light clothing is disregarded. Special features of the EFSA model like dense cultures, wearing of rain suits, etc., are not implemented in OWB as these are considered uncommon in amateur settings.

The contributing scenario covers the mixing and loading of the plant protection product into a hand-held sprayer. PPP can be a liquid, granular or powder formulation.

The contributing scenario also covers the dispersion of the diluted PPP using a hand-held sprayer. Spraying to high targets has a higher potential for exposure than spraying to low targets and therefore is considered as worst case. The indoor use of PPP by amateurs is considered as the reasonable worst-case in this contributing scenario; the outdoor use of such products is therefore not assessed.

**Table 11:** Typical CLE OWB output table (PC27) for GES3 showing exposure estimates for two tasks, one of which is associated with the handling of powder, granular, or liquid products. The subsequent task involves spraying of the typically diluted formulation (in water).

Type of equipment and conditions	Model	Formulation type	Dermal exposure [mg/kg bw/day]	Inhalation Exposure [mg/m <sup>3</sup> ]	Total RCR
Mixing and loading hand-held sprayer, indoors	BBA	Liquid	0.012	0.00029	0.0124
		Granule (WG)	0.012	0.00029	0.0124
		Powder (WP)	0.012	0.00029	0.0124
Hand-held spraying, high-level target, indoors		Liquid	0.885	0.0025	0.8874

An example of how combined exposure from the “sentinel” mixing and loading sub-activity, and spraying, is presented in the CSR is given in the following **Table 12**. The combined exposure is carried forward for risk assessment.

**Table 12:** Combined exposure estimates and RCRs for the loading of plant protection products into delivery equipment, as well as the spray application. This value is carried forward for use in risk characterisation, as a conservative estimate for this activity.

Sub-activities	Use rate		Dermal exposure [mg/kg bw/day]	Inhalation Exposure [mg/m <sup>3</sup> ]	Dermal RCR	Inhalation RCR	Total RCR
	[kg/ha]	[g/d]					
Task 1: Mixing & loading liquid formulation into knapsack sprayer	1.93	39	0.012	0.0003	0.012	0.0003	0.0124
Task 2: Hand-held spraying,			0.885	0.0025	0.885	0.0025	0.887

indoors						
<b>Task 1 + 2</b>		<b>0.897</b>	<b>0.003</b>	<b>0.897</b>	<b>0.0028</b>	<b>0.900</b>

### 2.5.5 PPP GES 4 - Use as a co-formulant in plant protection products, seed and granular applications by consumers

#### 2.5.5.1 Description of the activities and technical processes covered in the exposure scenario:

This exposure scenario covers the consumer use of a co-formulant in PPP, applied as granular formulation or treated seeds. This scenario includes both indoor and outdoor use.

This generic exposure scenario covers the following tasks:

- manual spreading by hand/spoon/cup, push rotary spreader, or belly grinder, of granular PPP or treated seeds on residential lawns/turf, gardens (flowers, fruits, vegetables), and trees (fruits, nuts, shrubs, ornamentals).

#### 2.5.5.2 Consumer contributing scenario 1: "Manual spreading of granular plant protection products or treated seeds"

Consumer use of granular PPP or treated seeds can take place with unprotected hands, using implements (spoons, cups), or by mechanical dispersion equipment, such as push-type rotary spreaders, or belly grinders.

The consumer use of PPP predominantly results in dermal and inhalation exposure. Oral exposure to granular PPP or treated seeds can result from inhalation of the non-respirable dust fraction which is eventually swallowed. Since the model data for inhalation include the respirable as well as the non-respirable dust fraction, the risk assessment for the inhalation route inherently covers this route of oral exposure as well. Direct oral intake of PPP is considered to be accidental and beyond a reasonable worst-case scenario.

Consumer exposure from these applications is assessed using the US EPA's Standard Operating Procedures for Residential Exposure Assessments (SOPREA)<sup>3</sup> using Equation 9 and Equation 10, assuming 100% absorption, as modified below:

$$E_{\text{dermal}} = AR \times A \times UE_{\text{route}} / (BW \times Cf) \quad \text{Equation 9}$$

$$E_{\text{inh}} = AR \times A \times UE_{\text{route}} / (RV \times Cf) \quad \text{Equation 10}$$

Where:

- $E_{\text{dermal}}$  = Dermal exposure, systemic (mg/kg bw)
- $E_{\text{inh}}$  = Inhalation exposure (mg/m<sup>3</sup>)
- $AR$  = Application rate (kg/ha)
- $A$  = Area (ha)
- $UE_{\text{route}}$  = Unit exposure for the relevant route and quantity handled (µg/lb)
- $BW$  = Body weight (kg)

<sup>3</sup> US Environmental Protection Agency - Standard Operating Procedures (SOPs) for Residential Exposure Assessments, Feb 2012, p. 3-3, available at [http://www.epa.gov/opp00001/science/EPA-OPP-HED\\_Residential%20SOPS\\_Feb2012.pdf](http://www.epa.gov/opp00001/science/EPA-OPP-HED_Residential%20SOPS_Feb2012.pdf) (accessed 8 Jun 2012))

- $RV$  = Respiratory volume ( $m^3$ )
- $C_f$  = lb to kg conversion factor (kg/lb)

The area per day that can be treated by manual/mechanical dispersion is  $200 m^2$ . As default it is assumed in this contributing scenario that no protective clothes are worn, i.e., consumers wear light clothes consisting of T-shirt and shorts. It is anticipated that one application per day takes place.

**Table 13:** Typical CLE OWB output table (PC27) for GES4 showing exposure estimates for five potential tasks involving mechanical or manual spreading of granular plant protection products or treated seeds. The worst-case "sentinel" value is highlighted in bold.

Type of equipment and conditions	Model	Formulation type	Dermal exposure [mg/kg bw/day]	Inhalation Exposure [mg/m <sup>3</sup> ]	Total RCR
"Push-type" Spreaders	SOPREA*	Solid (GR)	0.005	0.0000	0.005
Belly grinders			0.144	0.0007	0.144
Hand dispersal, spoon			0.035	0.0015	0.036
Hand dispersal, cup			0.001	0.0002	0.001
Hand dispersal			0.894	0.0064	<b>0.900</b>

\*SOPREA: US EPA SOP for Residential Exposure Assessments, Feb. 2012

## **2.6 CLE OWB - Frequently asked questions**

### **Q: I have dermal absorption data for my substance. Where can I enter these?**

A: Dermal absorption is not accounted for and is not required within CLE OWB. Using the DNEL concept, dermal absorption should be accounted for when setting dermal DNELs. Only external exposures are suitable for comparison with DNELs. This is a fundamental difference to the AOEL approach which is used for active substances under PPP legislation. The DNEL concept is akin to the route-specific MoE approach.

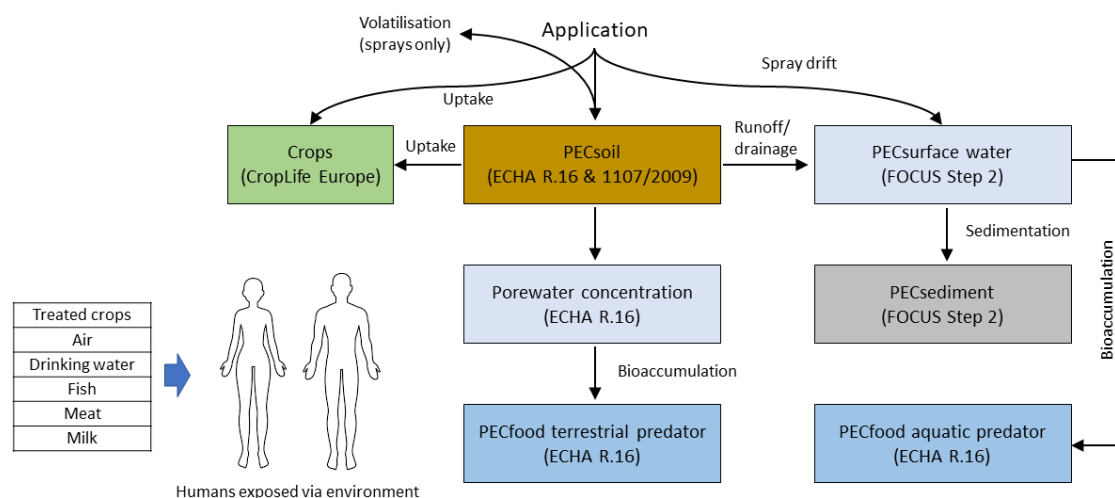
## **3 Environment: The CLE REACH-IN Local Environment Tool (LET) and the CLE SpERCs**

### **3.1 Introduction**

The environmental risk assessment for co-formulants used in agrochemical plant protection products should be conducted in two steps. The first step is to generate regional predicted environmental concentrations (PECs), associated with the use of the substance as a co-formulant in plant protection products (PPP) and its other uses in other life cycle stages. The second step is to conduct a local scale assessment of environmental exposure for just for the co-formulant use. The local scale assessment generates local concentrations for each relevant compartment that are then combined with the regional PECs to generate local PECs to be used in the risk characterisation.

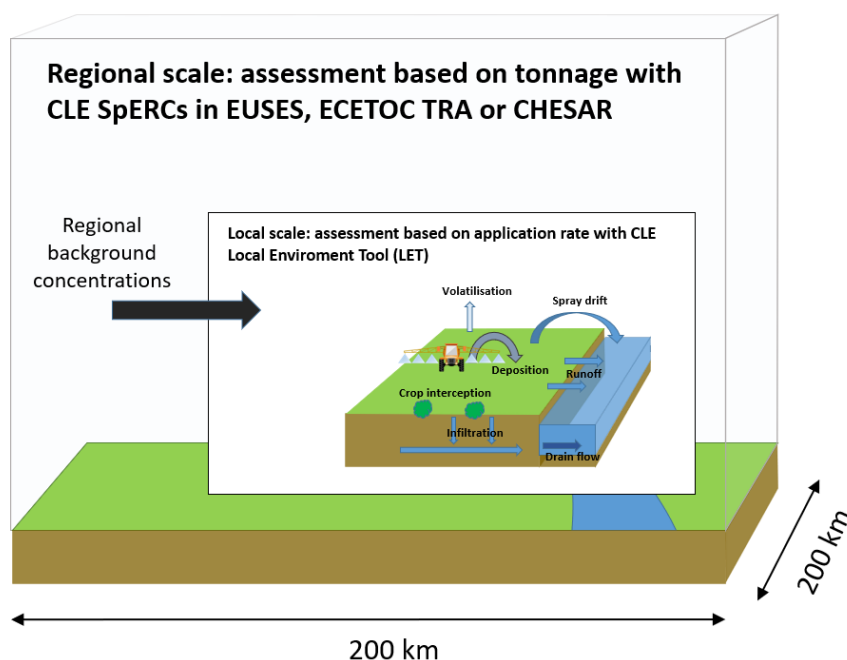
Regional scale estimates should be calculated outside the LET with appropriate tools, such as ECETOC TRA, EUSES or Chesar using the defined emission factors of the CLE Specific Environmental Release Categories (SpERCs) and can be imported into CLE Local Environment Tool (LET).

The LET calculates local-scale environmental concentrations and combines with regional PECs to perform risk characterisations which conform to the requirements of REACH. The LET is a simple spreadsheet tool which facilitates quantitative local-scale assessments for all REACH relevant environmental compartments (including soil and surface water, secondary poisoning via the food chain and indirect exposure of man via the environment). Conceptually, a treated 1 ha agricultural field with an adjacent shallow waterbody is simulated. Specifically, the LET uses the calculations described in the REACH R.16 (2016) guidance that is mostly based on the EU Technical Guidance Document on Risk Assessment (EU-TGD, 2003), as well as the Step 2 calculation approach for surface water devised by the Forum for the Co-ordination of pesticides fate models and their use (FOCUS, 2003). The calculation approach is illustrated below:

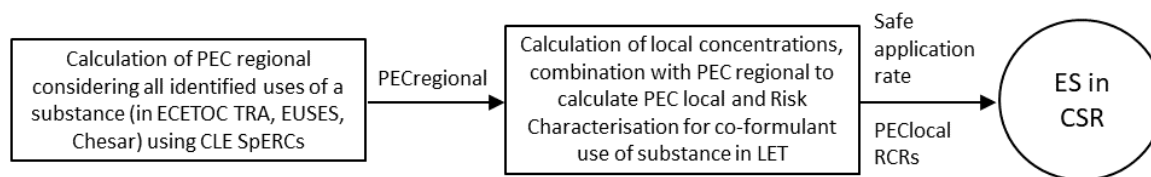


The calculations used in the LET for these assessments are discussed in detail in Section 3.6 (Model information & user guidance).

This scenario design is closely analogous to the established Tier 1 scenario used in the assessment of PPP active substances in the EU. It is considered to be a more appropriate representation of co-formulant uses than the industrial or municipal local settings implemented in the standard REACH models, and can be represented as:



The local scale assessment is conducted using an application rate approach (in contrast to the regional assessment which is conducted using a tonnage-based approach). The safe application rate, assumed conditions of use and the results of the risk characterisation are then included in the CSR, as summarised here:



It is foreseen that the LET will have two potential groups of users: Manufacturers/Importers (MI) and Downstream users (DU). In this context, MI's manufacture or import the substance of interest and register its uses, whilst DU's are plant protection product manufacturers. It is expected that the LET will be used in different ways, depending on the user.

MI users may know that a substance is used as a co-formulant but are unlikely to have detailed knowledge of how the co-formulant is used. Therefore, it is expected that these users will mainly perform a 'Default' assessment, taking account of a default realistic worst-case scenario (crop, region and timing of application) to determine a maximum total safe application rate (in kg/ha) that can be communicated to DU's via the extended safety data sheet (eSDS).

Alternatively, an assessment can be performed using the 'Refinement Options'. However, due to the level of understanding required and of the very restrictive nature of the conditions of use imposed on the substance's use, the option 'Assessment Type: Refinement Options' should only be used in close collaboration with all DU's manufacturing plant protection products.

On the other hand, upon receipt of the eSDS, DU's will be able to evaluate whether the existing LET assessment covers their specific representative use pattern of products containing the substance of interest or refine the assessment (using the Assessment Type: Refinements Options) by scaling, or as part of a DU Chemical Safety Report (DU CSR).

To facilitate scaling, it is recommended that the following text be incorporated into section 4 of exposure scenarios communicated to Downstream Users:

"The above exposure scenario may be scaled using the CLE Local Environment Tool (version 4.0) and using the parameters: co-formulant application rate, number of applications, application interval, crop (drift rate), location and period of application."

### 3.2 Parameterising the LET

All physical properties of the substance, as well as PNEC values, are required before the tool can be run. In many cases, manual entry of this substance-specific information into the LET will be necessary. Cells with required data are coloured yellow. Cells that contain optional or derived data are coloured blue. By default, the tool assumes the user will use the biodegradability classification to estimate the DT<sub>50</sub> values. However, if the experimental values are known these should be manually entered into the tool to maintain consistency with the values reported in the registration dossier. Selecting 'Don't use biodegradability classification' in the biodegradability classification dropdown list will change the DT<sub>50</sub> input to 'Manual input', after which the user can enter values in the appropriate boxes. DT<sub>50</sub> values in the 'Input' tab are assumed to be at 20 °C and measured values entered via 'Manual Input' should also be entered at 20 °C. The LET selects the option 'Don't use QSAR for K<sub>OC</sub>' on the QSAR dropdown list by default, and the user needs to manually enter an experimental K<sub>OC</sub> value. If such a value is not available, one of the QSARs listed in EU TGD and implemented in LET can be used to derive an estimated K<sub>OC</sub> value. In such a case, it is however required to provide a justification in the REACH dossier for using a calculation method to determine the K<sub>OC</sub> value.

Substance-specific information can be entered into the LET by importing it from an existing ECETOC TRA workbook if this is available. On clicking 'Import from ECETOC TRA' the user is asked to navigate to the required ECETOC TRA file. The tool then checks which substances are present in this file and allows the user to choose their substance from a drop-down list. The LET is then populated



with all the information that is present in the ECETOC TRA entry for this substance, including regional PEC, PNEC and DNEL values, where available. After import, values can still be changed manually; in some cases (e.g., DT<sub>50</sub> values) this may require changing the relevant dropdown from 'Import from ECETOC TRA' to 'Manual input'.

It should be noted that in the ECETOC TRA, regional PEC values are only recorded in an accessible form (and hence only extractable by the LET) if the ECETOC TRA has been run in 'batch' mode (see ECETOC TRA Manual). In brief, the ECETOC TRA can be run in two modes, 'manual' and 'batch'. The TRA is accessed via the ecetocTRAM.xls file, which has a number of tabs and opens with a set of 9 workbooks. The details for an individual substance can be entered into the INTERFACE tab, and the tool run in 'manual' mode using the 'run' button in cell E22. In this mode, the regional PEC values are not extractable. To run the ecetocTRAM tool in 'batch' mode (either cell E26 or one of the buttons in cell E27), it is first necessary to either directly enter substance/scenario data into the 'DATASHEETi' tab, or to transfer the data previously entered into the INTERFACE tab via the 'save' button in cell E24. Under these circumstances (i.e., in 'batch' mode) the Regional PEC values are written by the ECETOC TRA tool into the relevant 'DATASHEETi' tab, in rows 524-531. It is these values that are found and captured by the LET.

The LET will run without Regional PEC values being entered (zero values are assumed), but regional PECs should be included for runs generating risk characterisations for inclusion in the CSR.

For a 'Default' analysis the only parameter the user needs to define is whether the substance is applied as a spray treatment or a granule / seed treatment. During the 'Refinement Options' analysis there is more flexibility in the definition of the scenario. Keeping the default options ('No specific restrictions') for crop type and region and timing, selecting an interception of 0 and not including soil incorporation, will ensure the model is run for the reasonable worst-case scenario.

The model can be run if only the aquatic PNEC for a substance is entered. In this case, using the equilibrium partitioning method, expected PNEC values for the other compartments (with the exception of secondary poisoning) will be automatically calculated. However, if PNEC values derived from experimental data are available, these should be used.

### ***3.3 Running the LET***

Once all required values have been entered the 'Run' button will be activated. Model runs typically take less than a minute<sup>4</sup>, although this is dependent on the local system. It is recommended that the tool is run from a location on the local hard drive; running the tool over a network may reduce its speed significantly. The functionality of the tool cannot be guaranteed if it is launched directly from an e-mail attachment.

At the end of a model run, the output screen is shown. This screen shows a brief overview of the results generated using the scenario. Note the differences in model outputs discussed in Section 3.4 (Refinement options of the LET) and in Section 3.6 (Model information & user guidance). A fully documented set of results which can be included in a CSR document is available in the ExposureScenario tab.

Note: the tool is provided without any password protection; for reasons of transparency. However, users should be careful not to make any changes to the tool's code.

### ***3.4 'Refinement Options' of the LET***

Using the assessment type 'Default', the tool is run for a reasonable worst-case scenario, which is based on pre-selected input parameter values that were derived by an expert group appointed by the member companies of CropLife Europe (formerly European Crop Protection Association). The pre-selected input parameter values concern the region where a PPP is applied, the crop the substance is applied to

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<sup>4</sup> Note that running the LET on a laptop using battery power may see a significant drop in performance depending on the power saving options used.

and the timing of application. ‘Assessment Type: Default’ assumes a single application of the substance in a season (i.e., one application per year). At the end of a ‘Default’ assessment, an ‘Estimated Safe Dose’ is returned, and the RCR values for the environmental compartments are calculated using the local PECs calculated on the basis of this Estimated Safe Dose (note: by default, the Estimated Safe Dose is calculated using a maximum allowable RCR value of 0.90). Once this calculation step has been finished, there is an option to change the target RCR value on the output screen and selecting ‘refine dose’ results in a recalculation of the Estimated Safe Dose for that new RCR value. Effectively, the Estimated Safe Dose represents the maximum seasonal cumulated co-formulant application rate that passes the environmental assessment for all compartments. For a given substance, the LET should be run twice, once for its use in spray applications and once for its use in seed and granule applications. For downstream users, if the co-formulant dose arising from the use of a specific product is below the Estimated Safe Dose, then use in that product is considered covered by the exposure scenarios and CSA.

‘Assessment Type: Refinement Options’ gives the assessor the option to vary the scenario parameters to represent a specific situation of co-formulant use more closely. This includes varying the application rate, region and crop of application, timing of application and the number and frequency of applications, as well as the interception rate. At the end of a ‘Refinement Options’ analysis, the RCR values in each environmental compartment are returned based on the refine exposure scenario. In addition, an Estimated Safe Dose is calculated, but the model does not use this as an input at this point. By clicking ‘Refine Dose’ on the output sheet the model will be re-run for the scenario using the Estimated Safe Dose, should the user wish to explore the RCR values for this (note: the Estimated Safe Dose is calculated using a maximum allowable RCR value of 0.90). Once this has been calculated, there is an option to change the target RCR value on the output screen and selecting ‘refine dose’ results in a recalculation of the Estimated Safe Dose for that new RCR value. It should be noted that running the ‘Assessment Type: Refinement Options’ with the LET can result in a reduction of PECs in surface water if multiple applications are taken into account (due to reduced drift rates specified for multiple applications). Under these circumstances it is recommended that a single application is also simulated as this may represent the worst-case exposure via spray drift. The refinement options available for crop, type of interception, location and period of application are discussed in more detail in Section 3.6 (Model information & user guidance).

### ***3.5 Recommendations for assessment of difficult substances***

The LET employs equilibrium partitioning calculations from the EU-TGD. As a result, the same restrictions apply to this tool as to other EU-TGD-based tools such as the ECETOC TRA and Chesar. Specifically, the tool cannot necessarily be used for metals and metal substances, petroleum substances (UVCBs), polymeric and ionisable or ionic substances. Further guidance on how these types of substance should be assessed is provided in Appendix VIII, IX and XI of the EU-TGD Part 2, and ECHA R.7 appendices (2012).

#### ***3.5.1 Assessment of ionisable substances***

In particular, the LET can be used to screen for the risk associated with organic substances ionising at environmentally relevant pH values (i.e., in the range from 4-9). These substances ionise with change in the pH of the media (often to generate positively charged species; cations), such that at some pH values they are neutral, whereas at other pH values they are fully ionised (at interim pH values the substance is present as a mixture of ionised and neutral forms). There is usually a large difference in the environmental behaviour between the ionised and neutral forms of a substance. Neutral species usually adsorb much more strongly to solid media (e.g., soil, sediment, plants) and have a much higher tendency to partition into hydrophobic compartments; they also tend to be more volatile. Ionised species tend to strongly partition into aqueous phases.

A more detailed discussion on the environmental exposure assessment of ionisable organic compounds is available in the ECETOC Technical Report No. 123 ([ECETOC - Publications](#), 2013).

The LET can be used to investigate the risk arising from the neutral and ionised forms of the substance separately, by selecting input parameters that represent the behaviour of each specific species. Most of

the methods commonly used to generate the input data are designed to measure endpoints for the neutral species, and data for the ionised species are less likely to be available. However, worst case values for the ionised species can often be envisaged (e.g., a vapour pressure of zero, and a  $K_{OW}/K_{OC}$  of zero).

Consequently, in the first instance, it is recommended that two separate LET scenarios are explored; one for each species: neutral and ionised. For the neutral species, the LET run should use all the data available for the substance (ensuring that this is for predominantly the neutral species) and assuming that the substance is present 100% as the neutral species. For the ionised species, the LET run should be parameterised with a vapour pressure of  $1 \times 10^{-10}$  Pa and a  $K_{OW}/K_{OC}$  of zero. This is a worst case. The worst case RCRs for each compartment across the results from the two runs constitute the screening level assessment, and the maximum safe application rate should then be compared to the application rates associated with the use of the co-formulant.

If safety at the required application rates cannot be demonstrated, then possible refinements include integrating a more realistic understanding of the behaviour of the substance into the risk assessment. For example, when the  $pK_a$  is known, it is possible to calculate the proportion of each species (neutral or ionised) present at a given pH value. The toxicity of the two species is often very different, with the ionised species often being much less toxic (and such pH specific toxicity data could be obtained by experiment). Some ionised species, for example some cations, are strongly adsorbed to the clay components of soil. The variation of  $K_{OC}$  can also be measured experimentally in soils with different pH values, and these values could be used in the LET for pH specific runs. The  $K_{OW}$  can also be replaced in the LET for pH specific runs, with experimentally determined (or calculated)  $D_{OW}$  values (these are octanol-water distribution ratios, which are a measure of  $K_{OW}$  that accounts for the pH dependency of an ionisable organic chemical and is a measure of the distribution of ionised and neutral species in octanol and water as a function of pH).

The assessor needs to be aware of the complexity in this area; for example, partitioning of an ionised species to hydrophobic media can occur via ion-pairing, or if the substance has a significant hydrophobic component.

Where this screening approach indicates there may be unacceptable risk (even after considering possible refinements), then it might be necessary to seek alternative modelling approaches (e.g., MAMI III: Franco & Trapp, 2010).

### **3.6 Model information & user guidance**

#### **3.6.1 Input data**

Data requirements for co-formulants under REACH will depend on the substance properties and also the tonnage band for the substance. While certain studies on environmental fate parameters (e.g., measured soil adsorption ( $K_{OC}$ ) and measured soil, sediment, surface water degradation rates) may not be triggered as part of a co-formulant registration, these substance properties are key input parameters to estimate environmental exposure.

The CLE LET includes simple models that allow estimation of the key environmental parameters (i.e.,  $K_{OC}$ ,  $DT_{50}$  soil,  $DT_{50}$  sediment and  $DT_{50}$  surface water) where measured data are not available. These models are standard models and are included in other environmental exposure models such as EUSES and ECETOC TRA.

Predicted no effect concentrations (PNECs) for aquatic, sediment and soil compartments are also required. If a secondary poisoning assessment is necessary, a  $PNEC_{\text{secondary poisoning}}$  will be required. Where PNECs derived from experimental data are not available, these can be estimated for sediment and soil compartments via the equilibrium partitioning method.

General population DNELs (systemic effects, long term) for inhalation and oral routes are optional. The assessment of indirect exposure of humans via environment will run without these values, however, if DNELs are not entered this route will not be considered in the safe dose calculation.

### 3.6.1.1 $K_{OC}$ estimation

The user should enter a value for the soil adsorption ( $K_{OC}$ ) in the LET. By default, the ‘Don’t use QSAR for KOC’ option is selected in the tool, i.e., the assessor has to enter an experimental  $K_{OC}$  value, or a value that has been obtained with an appropriate estimation method. In the absence of such a value, the  $K_{OC}$  can be estimated using a Quantitative Structure Activity Relationship (QSAR). Several QSAR models for estimating soil adsorption are available and the most appropriate model will be dependent on the class of chemical assessed. The model developed by Sabljic and Güsten (1995) which estimates  $K_{OC}$  according to  $K_{OW}$  for up to 19 chemical classes, has been included in the LET, in line with EUSES and ECETOC TRA. The QSAR for different chemical classes is summarised in Table 14. As with any QSAR approach, the user should take care to select the most appropriate chemical class to allow a reasonable estimation of soil sorption.

**Table 14:** QSARs for soil sorption according to chemical class (Sabljic and Güsten, 1995)

Chemical Class	Equation
Predominantly hydrophobics	$\log K_{OC} = 0.81 \log K_{OW} + 0.10$
Nonhydrophobics	$\log K_{OC} = 0.52 \log K_{OW} + 1.02$
Phenols, anilines, benzo-nitriles, nitrobenzenes	$\log K_{OC} = 0.63 \log K_{OW} + 0.90$
Acetanilides, carbamates, esters, phenylureas, phosphates, triazines, triazoles, uracils	$\log K_{OC} = 0.47 \log K_{OW} + 1.09$
Alcohols, organic acids	$\log K_{OC} = 0.47 \log K_{OW} + 0.50$
Acetanilides	$\log K_{OC} = 0.40 \log K_{OW} + 1.12$
Alcohols	$\log K_{OC} = 0.39 \log K_{OW} + 0.50$
Amides	$\log K_{OC} = 0.33 \log K_{OW} + 1.25$
Anilines	$\log K_{OC} = 0.62 \log K_{OW} + 0.85$
Carbamates	$\log K_{OC} = 0.37 \log K_{OW} + 1.14$
Dinitroanilines	$\log K_{OC} = 0.38 \log K_{OW} + 1.92$
Esters	$\log K_{OC} = 0.49 \log K_{OW} + 1.05$
Nitrobenzenes	$\log K_{OC} = 0.77 \log K_{OW} + 0.55$
Organic acids	$\log K_{OC} = 0.60 \log K_{OW} + 0.32$
Phenols, benzonitriles	$\log K_{OC} = 0.57 \log K_{OW} + 1.08$
Phenylureas	$\log K_{OC} = 0.49 \log K_{OW} + 1.05$
Phosphates	$\log K_{OC} = 0.49 \log K_{OW} + 1.17$
Triazines	$\log K_{OC} = 0.30 \log K_{OW} + 1.50$
Triazoles	$\log K_{OC} = 0.47 \log K_{OW} + 1.41$

### 3.6.1.2 Biodegradation rates

It is expected that for the majority of substances only screening data on biodegradation (e.g., ready or inherent biodegradability tests) will be available. Conservative biodegradation rates in soil, surface water and sediment can be estimated from the results of the biodegradability screening tests. The ECHA R.16 guidance (2016) and EU-TGD report (2003) inferred half-lives for biodegradation in surface water are summarised in Table 15.

**Table 15:** Half-lives for biodegradation in surface water inferred on basis of biodegradability screening results (ECHA R.16 guidance and EU-TGD) at 12 °C

Test result	Half-life (days)
Readily biodegradable	15
Readily biodegradable, failing 10 day window	50
Inherently biodegradable	150
Not biodegradable	$\infty$

Inferred half-lives for biodegradation in soil and sediment are both partly dependent on partitioning, and the inferred half-life in sediment is a factor of 10 higher than in soil due to anoxic layers. The inferred half-lives for soil and sediment biodegradation reported in the ECHA R.16 (2016) and EU-TGD (2003) are summarised in Table 16 and Table 17.

**Table 16:** Half-lives for biodegradation in soil at 12 °C inferred on basis of biodegradability screening results (taken from ECHA R.16 guidance (2016) and EU-TGD (2003))

Kpsoil (L/kg)	Readily biodegradable (DT <sub>50</sub> , days)	Readily biodegradable, failing 10 day window (DT <sub>50</sub> , days)	Inherently biodegradable (DT <sub>50</sub> , days)	Not biodegradable (DT <sub>50</sub> , days)
<100	30	90	300	1.00E+06
>100, <1000	300	900	3000	1.00E+06
>1000, <10000	3000	9000	30000	1.00E+06
>10000	30000	90000	300000	1.00E+06

Kpsoil = K<sub>OC</sub> \* fraction organic carbon in standard soil (0.02)

**Table 17:** Half-lives for biodegradation in sediment at 12 °C inferred on basis of biodegradability screening results (taken from ECHA R.16 guidance (2016) and EU-TGD (2003))

Kpsoil (L/kg)	Readily biodegradable (DT <sub>50</sub> , days)	Readily biodegradable, failing 10-day window (DT <sub>50</sub> , days)	Inherently biodegradable (DT <sub>50</sub> , days)	Not biodegradable (DT <sub>50</sub> , days)
<100	300	900	3000	1.00E+07
>100, <1000	3000	9000	30000	1.00E+07
>1000, <10000	30000	90000	300000	1.00E+07
>10000	300000	900000	3000000	1.00E+07

Kpsoil = K<sub>OC</sub> \* fraction organic carbon in standard soil (0.02)

It should be noted that in the LET, the maximum DT<sub>50</sub> in soil, sediment and surface water has been limited to 1000 days, because this is the worst-case value which is used by the underlying FOCUS models.

When degradation is inferred from the biodegradability screening results in the LET, the DT<sub>50</sub> values are reported at 20 °C as this is the standard temperature used by the underlying FOCUS calculations. Therefore, when manually entering DT<sub>50</sub> values into the LET for soil, sediment or surface water, the values should also be for degradation at 20 °C. In the LET, the surface water and sediment DT<sub>50</sub> values at 20 °C are used directly to calculate the PEC in surface water and sediment, in accordance with the FOCUS (2003) algorithms. However, the DT<sub>50</sub> in soil is converted to the standard outdoor temperature of 12 °C, in accordance with the EU-TGD (2003) and ECHA R.16 (2016) guidance. The temperature

conversion of soil DT<sub>50</sub> from test temperature (20 °C) to environmental temperature (12 °C) is calculated according to Equation 11, in accordance with the EU-TGD (2003) and ECHA R.16 (2016) guidance.

$$DT_{50soil12^{\circ}C} = DT_{50soil20^{\circ}C} \times e^{(0.08 \times (20 - 12))} \quad \text{Equation 11}$$

Explanation of symbols

$DT_{50soil20^{\circ}C}$	Half-life of the co-formulant in soil at 20 °C	[d]	User input
$DT_{50soil12^{\circ}C}$	Half-life of the co-formulant in soil at environmental temperature	[d]	

The inferred degradation rates at 20 °C for soil, surface water and sediment reported in the “Input” tab of the LET are summarised in Table 18 to Table 20.

**Table 18:** Inferred Surface water degradation rates at 20 °C reported in the LET on basis of biodegradability screening results and FOCUSsw guidance

Test result	Half-life (days)
Readily biodegradable	7.91
Readily biodegradable, failing 10 day window	26.36
Inherently biodegradable	79.09
Not biodegradable	1000

**Table 19:** Inferred Soil degradation rates at 20 °C reported in the LET on basis of biodegradability screening results and FOCUSsw guidance

Kpsoil (L.kg <sup>-1</sup> )	Readily biodegradable (DT <sub>50</sub> , days)	Readily biodegradable, failing 10-day window (DT <sub>50</sub> , days)	Inherently biodegradable (DT <sub>50</sub> , days)	Not biodegradable (DT <sub>50</sub> , days)
<100	15.82	47.46	158.2	1000
>100, <1000	158.2	474.6	1000	1000
>1000, <10000	1000	1000	1000	1000

Kpsoil = K<sub>OC</sub> \* fraction organic carbon in standard soil (0.02)

**Table 20:** Inferred Sediment degradation rates at 20 °C reported in the LET on basis of biodegradability screening results and FOCUSsw guidance

Kpsoil (L.kg <sup>-1</sup> )	Readily biodegradable (DT <sub>50</sub> , days)	Readily biodegradable, failing 10-day window (DT <sub>50</sub> , days)	Inherently biodegradable (DT <sub>50</sub> , days)	Not biodegradable (DT <sub>50</sub> , days)
<100	158.2	474.6	1000	1000
>100, <1000	1000	1000	1000	1000

>1000, <10000	1000	1000	1000	1000
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$K_{psoil} = K_{OC} * \text{fraction organic carbon in standard soil (0.02)}$

### 3.6.1.3 PNEC derivation

#### PNEC Sediment derivation via equilibrium partitioning

In the LET, the PNEC for freshwater sediment can be estimated using the equilibrium partitioning method as described in the ECHA R.10 guidance (2008) and in Equation 12 to Equation 14.

$$K_{p_{susp}} = K_{OC} \times F_{OC_{susp}} \quad \text{Equation 12}$$

$$K_{susp-water} = F_{water_{susp}} + F_{solid_{susp}} \times K_{p_{susp}} / 1000 \times RHO_{solid} \quad \text{Equation 13}$$

$$PNEC_{sediment} = K_{susp-water} / RHO_{susp} \times PNEC_{sw} \times 1000 \quad \text{Equation 14}$$

#### Explanation of symbols

$K_{OC}$	Partition coefficient organic carbon -water	[L.kg <sup>-1</sup> ]	User input
$F_{OC_{susp}}$	Fraction organic carbon in the suspended solids	[-]	0.1
$F_{water_{susp}}$	Fraction water in suspended matter	[-]	0.9
$F_{solid}$	Fraction solid in suspended matter	[-]	0.1
$RHO_{solid}$	Bulk density of solid phase	[kg.m <sup>-3</sup> ]	2500
$PNEC_{sw}$	Predicted no effect concentration in freshwater	[mg.L <sup>-1</sup> ]	User input
$RHO_{susp}$	Bulk density of wet suspended matter	[kg.m <sup>-3</sup> ]	1150
$K_{p_{susp}}$	Partition coefficient solid-water in suspended matter	[L.kg <sup>-1</sup> ]	
$K_{susp-water}$	Suspended matter-water partition coefficient	[m <sup>3</sup> .m <sup>-3</sup> ]	
$PNEC_{sediment}$	Predicted no effect concentration in sediment (wet weight)	[mg.kg <sub>wwt</sub> <sup>-1</sup> ]	

Where the equilibrium partitioning method has been used to calculate the PNEC sediment and the log Kow is greater than 5, an additional assessment factor of 10 is applied to the RCR in sediment. This is to account for uptake via ingestion of sediment and is in line with the approach outlined in ECHA Part E guidance (2016).

#### PNEC Marine water derivation

Where the PNEC for marine water is not entered into the LET, the  $PNEC_{\text{marine water}}$  is assumed to be 1/10<sup>th</sup> of the PNEC for freshwater. This follows the ECHA R.10 guidance (2008) for marine water PNEC derivation, which recommends using an assessment factor that is 10 times greater than that used for freshwater. This is to account for uncertainty extrapolating freshwater effects to marine water environments.

$$PNEC_{\text{marine water}} = PNEC_{\text{surfacewater}} / 10 \quad \text{Equation 15}$$

#### Explanation of symbols

$PNEC_{\text{surface water}}$	Predicted no effect concentration in freshwater	[µg.L <sup>-1</sup> ]	User input
$PNEC_{\text{marinewater}}$	Predicted no effect concentration in marine water	[µg.L <sup>-1</sup> ]	

PNEC Marine water sediment derivation

Where the PNEC in marine water sediment is not entered into the LET, the  $PNEC_{\text{marine sediment}}$  is estimated from the  $PNEC_{\text{marine water}}$  via the equilibrium partitioning method.

$$PNEC_{\text{marine sediment}} = K_{\text{susp-water}} / RHO_{\text{susp}} \times PNEC_{\text{marine water}} \times 1000 \quad \text{Equation 16}$$

## Explanation of symbols

$K_{\text{susp-water}}$	Suspended matter-water partition coefficient	[m <sup>3</sup> .m <sup>-3</sup> ]	Equation 13
$RHO_{\text{susp}}$	Bulk density of wet suspended matter	[kg.m <sup>-3</sup> ]	1150
$PNEC_{\text{marinewater}}$	Predicted no effect concentration in marine water	[mg.L <sup>-1</sup> ]	User input or Equation 15
$PNEC_{\text{marine sediment}}$	Predicted no effect concentration in marine sediment (wet weight)	[mg.kg <sub>wwt</sub> <sup>-1</sup> ]	

Where the equilibrium partitioning method has been used to calculate the PNEC marine water sediment and the log Kow is greater than 5, an additional assessment factor of 10 is applied to the RCR in marine water sediment. This is to account for uptake via ingestion of sediment and is in line with the approach outlined in ECHA Part E guidance (2016).

PNEC sediment conversion from wet weight to dry weight

The  $PNEC_{\text{sediment}}$  and  $PNEC_{\text{marine sediment}}$  can be entered into the LET manually either in mg.kg<sub>dwt</sub><sup>-1</sup> or in mg.kg<sub>wwt</sub><sup>-1</sup>. These units are converted using the following calculation:

$$PNEC_{\text{sed}_{\text{dwt}}} = PNEC_{\text{sed}_{\text{wwt}}} \times CONV_{\text{susp}} \quad \text{Equation 17}$$

$$CONV_{\text{susp}} = RHO_{\text{susp}} / (F_{\text{solid}_{\text{susp}}} \times RHO_{\text{solid}}) \quad \text{Equation 18}$$

## Explanation of symbols

$PNEC_{\text{sed}_{\text{wwt}}}$	Predicted No effect concentration in sediment (wet weight)	[mg.kg <sub>wwt</sub> <sup>-1</sup> ]	User input
$CONV_{\text{susp}}$	Conversion factor for suspended matter concentration: wwt to dwt	[kg <sub>wwt</sub> .kg <sub>dwt</sub> <sup>-1</sup> ]	Equation 18
$RHO_{\text{susp}}$	Wet bulk density of suspended matter	[kg <sub>wwt</sub> .m <sup>-3</sup> ]	1150
$F_{\text{solid}_{\text{susp}}}$	Volume fraction of solids in suspended matter	[m <sup>3</sup> .m <sup>-3</sup> ]	0.1
$RHO_{\text{solid}}$	Bulk density of solids	[kg <sub>dwt</sub> .m <sup>-3</sup> ]	2500
$PNEC_{\text{sed}_{\text{dwt}}}$	Predicted No effect concentration in sediment (dry weight)	[mg.kg <sub>dwt</sub> <sup>-1</sup> ]	

PNEC Soil derivation via equilibrium partitioning

The  $PNEC_{\text{soil}}$  can also be estimated in the LET via the equilibrium partitioning method using Equation 19, in accordance with ECHA R.10 guidance (2008).

$$PNEC_{\text{soil}} = K_{\text{soil-water}} / RHO_{\text{soil}} \times 1000 \quad \text{Equation 19}$$



## Explanation of symbols

$PNEC_{sw}$	Predicted no effect concentration in freshwater	[mg.L <sup>-1</sup> ]	User input
$RHO_{soil}$	Bulk Density of wet soil	[kg.m <sup>-3</sup> ]	1700
$K_{soil-water}$	Soil-water equilibrium partition coefficient	[m <sup>3</sup> .m <sup>-3</sup> ]	Equation 37
$PNEC_{soil}$	Predicted no effect concentration in soil (wet weight)	[mg.kg <sub>wwt</sub> <sup>-1</sup> ]	

Where the equilibrium partitioning method has been used to calculate the PNEC soil and the log K<sub>ow</sub> is greater than 5, an additional assessment factor of 10 is applied to the RCR in soil. This is to account for uptake via ingestion of soil and is in line with the approach outlined in ECHA Part E guidance (2016).

PNEC soil conversion from wet weight to dry weight

The PNEC<sub>soil</sub> can be entered into the LET manually either in mg.kg<sub>dwt</sub><sup>-1</sup> or in mg.kg<sub>wwt</sub><sup>-1</sup>. These units are converted using the following calculation:

$$PNEC_{soil_{dwt}} = PNEC_{soil_{wwt}} \times CONV_{soil} \quad \text{Equation 20}$$

## Explanation of symbols

$PNEC_{soil_{wwt}}$	Predicted no effect concentration in soil (wet weight)	[mg.kg <sub>wwt</sub> <sup>-1</sup> ]	User input
$CONV_{soil}$	Conversion factor for soil concentration wet-dry weight soil	[kg <sub>wwt</sub> .kg <sub>dwt</sub> <sup>-1</sup> ]	Equation 92
$PNEC_{soil_{dwt}}$	Predicted no effect concentration in soil (dry weight)	[mg.kg <sub>dwt</sub> <sup>-1</sup> ]	

## 3.6.1.4 LET Assessment Type

The LET can be run using either an Assessment Type: ‘Default’ or ‘Refinement Options’. When the user selects the ‘Default’ assessment type, the only input required is to select the ‘Application Type’. A ‘Default’ assessment is intended to represent a realistic worst-case estimate of exposure, as defined for a range of parameters (crop, soil incorporation, interception type, region and timing of application). For soil incorporation, interception type, region and timing of application, the worst-case value was selected as the default for the ‘Default’ assessment scenario.

Crop type determines the drift percentage used in the surface water PEC calculation. For a ‘Default’ assessment ‘fruit (late)’ was selected (Table 26). It should be noted that some crops have higher drift rates than this (e.g., ‘fruit, early’). However, early applications are actually quite rare, since the trees have no foliage at that stage, so this value was rejected for use as a realistic ‘Default’. Similarly, the drift rate for aerial applications was also rejected as a realistic worst-case, since applications of this type now require a derogation within the EU, which cannot be considered to represent normal practice. The parameterisation of the ‘Default’ assessment is summarised in Table 21.

**Table 21:** Summary of ‘Assessment Type: Default’ parameterisation

Parameter	‘Default’ value	Justification
Crop	Pome/stone fruit late (15.7% drift)	Realistic worst-case
Soil incorporation	No (0.05 m mixing depth)	Default value used in plant protection product risk assessments
Interception type	No interception	Worst-case

Region and timing of application	N. Europe, Oct – Feb (5% of soil residue available for runoff)	Worst-case (See Table 27)
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It should be noted that selection of solid formulations automatically sets the drift percentage to zero. Where the ‘Refinement Options’ assessment mode is selected, the user can change any of the parameters discussed above, however, it should be noted that any changes from the ‘Default’ assessment type should be representative of all the intended uses of the co-formulant.

### 3.6.2 Soil model

The fraction of co-formulant reaching the soil surface is dependent on formulation type, vapour pressure and crop interception. Once the co-formulant reaches the soil surface it is assumed to be homogeneously mixed to 0.05 m (in accordance with the default value used in plant protection product risk assessments). The  $PEC_{soil}$  reported in the LET is calculated as a 30-day time weighted average, following 10-year annual applications and includes the removal processes of biodegradation, volatilisation and leaching, in accordance with the EU-TGD and ECHA R.16 guidance (2016). A 180-day time weighted average  $PEC_{soil}$  and a PEC in porewater are also calculated by the LET, but not reported in the “Output” tab. These PECs are used to calculate the  $PEC_{secondary\ poisoning}$  for terrestrial predators and used in the exposure to humans via environment assessment.

#### 3.6.2.1 Soil loading

For co-formulants included in spray formulations, the dose which reaches the soil can be significantly reduced due to volatilisation of spray droplets and by crop cover. Whereas for co-formulants included in seed treatments, the dose which reaches the soil will not be reduced, and for foliar applied granules will only be reduced by crop cover.

#### 3.6.2.2 Volatilisation of spray droplets

The emission fractions to air due to volatilisation are taken from the pesticides field application module in USES 4.0 (RIVM, VROM, VWS (2002)). Substances having a vapour pressure of  $>0.01$  Pa at environmental conditions are considered as volatile and assumed to evaporate completely from soil or plant leaf surfaces in a relatively short period of time. Therefore, the release factor for soil for these volatile substances is set to zero. For substances with lower vapour pressures, the release fraction to the soil compartment is set to one. More details on the generation of the emission fractions can be found in Dobe *et al.*, (2020). The emission fractions are summarised in Table 22, and it is assumed that these emission fractions apply for both indoor and outdoor use.

**Table 22:** Release to air and soil following volatilisation of sprays (Dobe *et al.*, (2020))

Vapour Pressure (Pa)	Total emission factor to air (-) $F_{air}$	Total emission factor to soil (-) $F_{soil}$
$>0.010$	1	0
$>0.001-0.010$	0.5	1
$>0.0001-0.001$	0.2	1
$0.00001-0.0001$	0.1	1
$<0.00001$	0.01	1

In order to determine emission to air under field conditions, the vapour pressure is corrected to a standard temperature of 25 °C using Equation 21.

$$VP(TEMP_{standard}) = VP(TEMP_{test}) \times e^{(H_{0vapour} / R \times (1 / (273 + TEMP_{test}) - 1 / (273 + 25)))}$$
 Equation 21

Explanation of symbols

$VP(TEMP_{test})$	Vapour Pressure as give in the data set	[Pa]	User input
$H_{0vapor}$	Enthalpy of vaporisation	[J/mol]	$5 \times 10^4$
$R$	Gas constant	[Pa.m <sup>3</sup> .mol <sup>-1</sup> .k <sup>-1</sup> ]	8.314
$TEMP_{test}$	Temperature at which vapour pressure was measured	[°C]	User input
$VP(TEMP_{standard})$	Vapour Pressure at standard temperature (25 °C)	[Pa]	

This emission factor to soil takes account of the volatilisation of spray droplets and, therefore, is not applicable when the application type is set to ‘granule application / seed treatment’. Where the application type is set to ‘granule application / seed treatment’, volatilisation during application is assumed to be zero. Volatilisation of the co-formulant from the soil compartment is accounted for in the LET and is discussed in Section 3.6.2.7.

### 3.6.2.3 Crop interception

The release factor to soil may be further reduced due to crop interception. For ‘Assessment Type: Default’, no crop interception is applied as a worst-case assessment of soil exposure (see Table 21). However, crop interception can be defined in ‘Refinement Options’, where interception will be dependent on crop and growth stage. The crop interception values presented in FOCUS surface water Step 2 (2003) were summarised in suitable generic crop categories (see Table 23) (these categories also define the spray-drift values). It is recommended to use this set of generic crop categories if a higher-tier refinement of the exposure assessment is necessary. Standard phrases for communication of exposure scenario information have been based on these crop categories.

**Table 23:** Crop interception values for twelve generic crop categories

Crop	No interception	$F_{crop}$ (interception fraction)		
		Minimal crop cover	Intermediate crop cover	Full canopy
BBCH-code	00 – 09	10 – 19	20 – 39	40 – 89
No drift (incorporation/seed treatment)	0	0	0	0
Spray to bare soil / pre-emergent use	0	0	0	0
Vegetable crops	0	0.1	0.25	0.4
Fruit (early)	0	0.2	0.4	0.7

Crop	No interception	F <sub>crop</sub> (interception fraction)		
		Minimal crop cover	Intermediate crop cover	Full canopy
Fruit (late)	0	0.2	0.4	0.7
Hand applications (crop < 50 cm)	0	0.2	0.5	0.7
Hand applications (crop > 50 cm)	0	0.2	0.5	0.7
Hops	0	0.2	0.5	0.7
Aerial application	0	0.2	0.5	0.7
Arable crops	0	0.25	0.5	0.7
Vines, early applications	0	0.4	0.5	0.7
Vines, late applications	0	0.4	0.5	0.7

The crop interception values from FOCUS surface water Step 2 (2003) for a more detailed list of crops are also implemented in the CLE LET and are summarised in Table 24. These may be used in the higher-tier assessment of local environmental exposure resulting from the use of plant protection products on specific crops.

**Table 24:** Crop interception values (FOCUS surface water Step 2)

Crop	No interception	F <sub>crop</sub> (interception fraction)		
		Minimal crop cover	Intermediate crop cover	Full canopy
BBCH-code	00 – 09	10 – 19	20 – 39	40 – 89
cereals, spring and winter	0	0.25	0.5	0.7
citrus	0	0.7	0.7	0.7
cotton	0	0.3	0.6	0.75
field beans	0	0.25	0.4	0.7
grass / alfalfa	0	0.4	0.6	0.75
hops	0	0.2	0.5	0.7
legumes	0	0.25	0.5	0.7
maize	0	0.25	0.5	0.75
oil seed rape, spring and winter	0	0.4	0.7	0.75
olives	0	0.7	0.7	0.7
pome / stone fruit, early and late	0	0.2	0.4	0.7
potatoes	0	0.15	0.5	0.7
soybeans	0	0.2	0.5	0.75
sugar beet	0	0.2	0.7	0.75
sunflower	0	0.2	0.5	0.75
tobacco	0	0.2	0.7	0.75
vegetables, bulb	0	0.1	0.25	0.4
vegetables, fruiting	0	0.25	0.5	0.7
vegetables, leafy	0	0.25	0.4	0.7
vegetables, root	0	0.25	0.5	0.7
Vines, early and late	0	0.4	0.5	0.7
application, aerial	0	0.2	0.5	0.7

Crop	No interception	F <sub>crop</sub> (interception fraction)		
		Minimal crop cover	Intermediate crop cover	Full canopy
application, hand (crop < 50 cm and > 50 cm)	0	0.2	0.5	0.7
no drift (incorporation /seed treatment)	0	0	0	0

### 3.6.2.4 Calculation of soil loading

The soil loading is calculated as the co-formulant application rate corrected for the fraction emitted to air through volatilisation of spray droplets and the fraction intercepted by crop cover. Where the assessment type is set to 'Default' only volatilisation (for sprays) is considered.

$$\text{Soil Loading} = \text{AR} \times F_{\text{soil}} \times (1 - F_{\text{crop}}) \quad \text{Equation 22}$$

#### Explanation of symbols

<i>AR</i>	Application rate for co-formulant	[g.ha <sup>-1</sup> ]	User input
<i>F<sub>crop</sub></i>	Fraction of interception by crop (refinement option)	[-]	Table 24
<i>F<sub>soil</sub></i>	Emission factor to soil due to volatilisation of spray droplets (spray only)	[-]	Table 22
<i>Soil Loading</i>	Soil loading of the co-formulant	[g.ha <sup>-1</sup> ]	

### 3.6.2.5 Concentration in soil

The concentration in soil is calculated by taking account of the application rate adjusted for the fraction emitted to soil and the fraction intercepted by crop cover, the soil mixing depth and bulk density. For a 'Default' assessment a mixing depth of 0.05 m is assumed (see Table 21), in accordance with the default value used in plant protection product risk assessments. The default for grassland (non-ploughed soil) in the REACH R.16 guidance (2012) is 0.10 m, however, this was not considered conservative for a co-formulant applied directly to untilled soil (e.g., orchards). In a refined assessment it is possible to take account of soil incorporation, if it is known that the co-formulant will be mixed into soil (e.g., by ploughing). To take account of this, a mixing depth of 0.20 m is assumed.

The PEC in soil is calculated as a 30-day time-weighted average following the last application event after 10 years of annual applications and includes losses through biodegradation, leaching and volatilisation. This approach is in accordance with the ECHA R.16 guidance (2016).

### 3.6.2.6 Initial concentration in soil after a single application

The initial concentration in soil after one application is calculated as the following:

$$C_{\text{soil,initial}} = \text{Soil Loading} \times 1000 / (\text{DEPTH}_{\text{soil}} \times \text{RHO}_{\text{soil}} \times 10000) \quad \text{Equation 23}$$

#### Explanation of symbols

<i>DEPTH<sub>soil</sub></i>	Mixing depth of soil	[m]	Default: 0.05 Incorporation: 0.20
<i>RHO<sub>soil</sub></i>	Bulk density of wet soil	[kg.m <sub>wwt</sub> <sup>-3</sup> ]	1700

<i>Soil Loading</i>	Soil loading of the co-formulant	[g.ha <sup>-1</sup> ]	Equation 22
10000	Area of 1 hectare	[m <sup>2</sup> ]	
<i>Csoil<sub>initial</sub></i>	Initial concentration in soil	[mg.kg <sub>wwt</sub> <sup>-1</sup> ]	

### 3.6.2.7 Maximum concentration in soil

In the case of a single application: the maximum concentration in soil in one year is expected to occur immediately following application. Therefore, the following applies:

$$C_{soil_{max\_1}} = C_{soil_{initial}} \quad \text{Equation 24}$$

In the case of multiple seasonal applications: the maximum concentration in soil is expected to occur after the last application. In between application events, it is assumed that losses due to degradation, volatilisation and leaching will occur. Losses due to degradation at environmental temperature (12 °C) are calculated according to Equation 25, losses due to volatilisation are calculated according to Equation 26 and losses due to leaching are calculated according to Equation 27. The equations describing loss processes are in accordance with ECHA guidance R.16.

$$k_{bio_{soil}} = \ln 2 / DT_{50_{bio_{soil}}} \quad \text{Equation 25}$$

#### Explanation of symbols

<i>DT<sub>50</sub><sub>bio<sub>soil</sub></sub></i>	Half-life for biodegradation in bulk soil at 12 °C	[d]	Equation 11
<i>k<sub>bio<sub>soil</sub></sub></i>	first order rate constant for biodegradation in bulk soil	[d <sup>-1</sup> ]	

$$1 / k_{volat} = ((1 / (kasl_{air} \times K_{air-water} / K_{soil-water}) + 1 / kasl_{soil}) \times DEPTH_{soil}) \quad \text{Equation 26}$$

#### Explanation of symbols

<i>kasl<sub>air</sub></i>	Partial mass transfer coeff. at air side of the air-soil interface	[m.d <sup>-1</sup> ]	90.72
<i>kasl<sub>soil</sub></i>	Partial mass transfer coeff. at soil-side of the air-soil interface	[m.d <sup>-1</sup> ]	See ECHA R.16 guidance (2016), Equation R.16-59
<i>K<sub>air-water</sub></i>	Air-water equilibrium distribution constant	[m <sup>3</sup> .m <sup>-3</sup> ]	Equation 39
<i>K<sub>soil-water</sub></i>	Soil-water partitioning coefficient	[m <sup>3</sup> .m <sup>-3</sup> ]	Equation 37
<i>DEPTH<sub>soil</sub></i>	Mixing depth of soil	[m]	Default: 0.05 Incorporation: 0.20
<i>k<sub>volat</sub></i>	Pseudo first-order rate constant for volatilisation from soil	[d <sup>-1</sup> ]	

$$k_{leach} = (Finf_{soil} \times RAIN_{rate}) / K_{soil-water} \times DEPTH_{soil} \quad \text{Equation 27}$$

## Explanation of symbols

$F_{inf,soil}$	Fraction of rainwater that infiltrates into soil	[-]	0.25
$RAINrate$	Rate of wet precipitation (700 mm/year)	[m.d <sup>-1</sup> ]	$1.92 \times 10^{-3}$
$K_{soil-water}$	Soil-water partitioning coefficient	[m <sup>3</sup> .m <sup>-3</sup> ]	Equation 37
$DEPTH_{soil}$	Mixing depth of soil	[m]	Default: 0.05 Incorporation: 0.20
$k_{leach}$	Pseudo-first order rate constant for leaching from soil layer	[d <sup>-1</sup> ]	

The overall rate constant for these removal processes is given in Equation 28.

$$k = k_{volat} + k_{leach} + k_{bio_{soil}} \quad \text{Equation 28}$$

## Explanation of symbols

$k_{volat}$	Pseudo-first order rate constant for volatilisation from soil	[d <sup>-1</sup> ]	Equation 26
$k_{leach}$	Pseudo-first order rate constant for leaching from top soil	[d <sup>-1</sup> ]	Equation 27
$k_{bio_{soil}}$	Pseudo-first order rate constant for biodegradation in soil	[d <sup>-1</sup> ]	Equation 25
$k$	First order rate constant for removal from top soil	[d <sup>-1</sup> ]	Equation 28

The maximum concentration in soil following multiple applications in one year is calculated with Equation 29.

$$C_{soil,max\_1} = C_{soil,initial} \times ((1 - e^{(-k \times App\ Int)^{N_{app}}}) / (1 - e^{(-k \times App\ Int)})) \quad \text{Equation 29}$$

## Explanation of symbols

$C_{soil,initial}$	Initial concentration in soil	[mg.kg <sub>wwt</sub> <sup>-1</sup> ]	Equation 23
$k$	First order rate constant for removal from top soil	[d <sup>-1</sup> ]	Equation 28
$App\ Int$	Application interval	[d]	User input
$N_{app}$	Number of application events	[-]	User input
$C_{soil,max\_1}$	Maximum concentration in soil in year 1	[mg.kg <sub>wwt</sub> <sup>-1</sup> ]	

To account for the potential of accumulation in soil following applications in subsequent years, annual application to soil for 10 years is calculated. The fraction accumulated in soil in one year is calculated with Equation 30.

$$F_{acc} = e^{-365 \times k} \quad \text{Equation 30}$$

## Explanation of symbols

$k$	First order rate constant for removal from top soil	[d <sup>-1</sup> ]	Equation 28
$F_{acc}$	Fraction accumulated in one year	[-]	

The maximum concentration in soil following the last application in year 10 is calculated with Equation 31.

$$C_{soil_{10}} = C_{soil_{max_{-1}}} \times (1 + \sum_{n=1}^9 F_{acc}^n) \quad \text{Equation 31}$$

## Explanation of symbols

$C_{soil_{max_{-1}}}$	Maximum concentration in soil in year 1	[mg.kg <sub>wwt</sub> <sup>-1</sup> ]	Equation 29
$F_{acc}$	Fraction accumulated in one year	[-]	Equation 30
$C_{soil_{10}}$	Maximum concentration in soil in year 10	[mg.kg <sub>wwt</sub> <sup>-1</sup> ]	

## 3.6.2.8 Time-weighted average concentration in soil

The time-weighted average concentration in soil over time period,  $t$ , is defined as:

$$TWAC_{soil}(t) = C_{soil_{10}} \times (1 - e^{(-k \times t)}) / (k \times t) \quad \text{Equation 32}$$

## Explanation of symbols

$C_{soil_{10}}$	Maximum concentration in soil in year 10	[mg.kg <sub>wwt</sub> <sup>-1</sup> ]	Equation 31
$k$	First order rate constant for removal from top soil	[d <sup>-1</sup> ]	Equation 28 Soil: 30
$t$	Time period	[d]	Secondary poisoning: 180 Humans via environment: 180
$TWAC_{soil}(t)$	Time weighted average concentration in soil, over a period $t$	[mg.kg <sub>wwt</sub> <sup>-1</sup> ]	

If application to soil will only take place once (i.e., no repeated annual applications), the annual application option can be set to 1 year. This option is not recommended unless it is known that the co-formulant will not be applied to soil in subsequent years. In this situation the time-weighted average concentration in soil over time period,  $t$ , is defined as:

$$TWAC_{soil}(t) = C_{soil_{max_{-1}}} \times (1 - e^{(-k \times t)}) / (k \times t) \quad \text{Equation 33}$$

## Explanation of symbols



$C_{soil_{max_1}}$	Maximum concentration in soil in year 1	$[\text{mg.kg}_{\text{wwt}}^{-1}]$	Equation 29
$k$	First order rate constant for removal from top soil	$[\text{d}^{-1}]$	Equation 28 Soil: 30
$t$	Time period	$[\text{d}]$	Secondary poisoning: 180 Humans via environment: 180
$TWAC_{soil}(t)$	Time weighted average concentration in soil, over a period $t$	$[\text{mg.kg}_{\text{wwt}}^{-1}]$	

In accordance with the EU-TGD (2003) and REACH R.16 guidance (2016), the time weighted average of 30 days has been considered appropriate for the local concentration in soil (Equation 34), rather than the 28 days used by default by FOCUS (2003).

$$C_{local_{soil}} = TWAC_{soil(30d)} \quad \text{Equation 34}$$

The local concentration in soil, as a time weighted average of 180 days, is also calculated in the LET but not used as the local concentration for the terrestrial compartment. Instead, the local concentration in soil at 180 days is used in the secondary poisoning assessment for terrestrial organisms and for the local scale assessment of humans exposed via the environment. This is discussed in more detail in Section 3.6.4 and Section 3.6.5, respectively.

$$C_{local_{soil,secondary\ poisoning}} = TWAC_{soil(180d)} \quad \text{Equation 35}$$

$$C_{local_{soil,humans\ via\ env}} = TWAC_{soil(180d)} \quad \text{Equation 36}$$

### 3.6.2.9 Porewater concentration

The LET also calculates the concentration in soil porewater. The soil porewater calculation is used to estimate the amount of substance available to earthworms via uptake from the soil porewater. This is used for the secondary poisoning assessment for terrestrial organisms which is discussed in more detail in Section 3.6.4. It is also used in the local scale assessment of humans exposed via the environment discussed in Section 3.6.5.

The concentration in porewater is calculated from the concentration in soil and the soil-water partitioning coefficient. For the secondary poisoning assessment and the local scale assessment of humans exposed via the environment, the time weighted average at 180 days is used. The soil-water partitioning coefficient is calculated according to Equation 37.

$$K_{soil-water} = F_{air_{soil}} \times K_{air-water} + F_{water_{soil}} + F_{solid_{soil}} \times K_{p_{soil}} / 1000 \times RHO_{solid} \quad \text{Equation 37}$$

Where:

$$K_{p_{soil}} = K_{oc} \times F_{oc_{soil}} \quad \text{Equation 38}$$

$$K_{air-water} = HENRY / (R \times TEMP) \quad \text{Equation 39}$$

$$\text{HENRY} = \text{VP}(\text{TEMP}_{\text{env}}) \times \text{MOLW} / \text{SOL}(\text{TEMP}_{\text{env}}) \quad \text{Equation 40}$$

## Explanation of symbols

$VP(\text{TEMP}_{\text{env}})$	Vapour Pressure at environmental temperature (12 °C)	[Pa]	Equation 42
$\text{SOL}(\text{TEMP}_{\text{env}})$	Solubility in water at environmental temperature (12 °C)	[mg.L <sup>-1</sup> ]	Equation 41
$\text{MOLW}$	Molecular weight	[g.mol <sup>-1</sup> ]	User input
$R$	Gas constant	[Pa.m <sup>3</sup> .mol <sup>-1</sup> .K <sup>-1</sup> ]	8.314
$\text{TEMP}$	Temperature at the air-water interface	[K]	285
$K_{OC}$	Partition coefficient organic carbon -water	[L.kg <sup>-1</sup> ]	User input
$F_{OC_{\text{soil}}}$	Fraction organic carbon in the soil	[-]	0.02
$F_{air_{\text{soil}}}$	Fraction air in soil	[-]	0.2
$F_{water_{\text{soil}}}$	Fraction water in soil	[-]	0.2
$F_{solid_{\text{soil}}}$	Fraction solid in soil	[-]	0.6
$RH_{O_{\text{solid}}}$	Bulk density of solids	[kg.m <sup>-3</sup> ]	2500
$\text{HENRY}$	Henry's law constant	[Pa.m <sup>3</sup> .mol <sup>-1</sup> ]	
$K_{air-water}$	Air-water partitioning coefficient	[-]	
$K_{p_{\text{soil}}}$	Solids-water partition coefficient in soil	[L.kg <sup>-1</sup> ]	
$K_{soil-water}$	Soil-water partitioning coefficient	[m <sup>3</sup> .m <sup>-3</sup> ]	

The water solubility and vapour pressure are converted from test temperature to environmental temperature using Equation 41 and Equation 42, respectively.

$$\text{SOL}(\text{TEMP}_{\text{env}}) = \text{SOL}(\text{TEMP}_{\text{test}}) \times e^{((H_{0_{\text{solut}}}/R) \times ((1/273 + \text{TEMP}_{\text{test}})^{-1} - (1/273 + 12)^{-1}))} \quad \text{Equation 41}$$

$$\text{VP}(\text{TEMP}_{\text{env}}) = \text{VP}(\text{TEMP}_{\text{test}}) \times e^{((H_{0_{\text{vapor}}}/R) \times ((1/273 + \text{TEMP}_{\text{test}})^{-1} - (1/273 + 12)^{-1}))} \quad \text{Equation 42}$$

## Explanation of symbols

$VP(\text{TEMP}_{\text{test}})$	Vapour Pressure at test temperature	[Pa]	User input
$H_{0_{\text{vapor}}}$	Enthalpy of vaporisation	[J.mol <sup>-1</sup> ]	5 × 10 <sup>4</sup>
$R$	Gas constant	[Pa.m <sup>3</sup> .mol <sup>-1</sup> .K <sup>-1</sup> ]	8.314
$\text{SOL}(\text{TEMP}_{\text{test}})$	Solubility in water at test temperature	[mg.L <sup>-1</sup> ]	User input
$H_{0_{\text{solut}}}$	Enthalpy of solution	[J.mol <sup>-1</sup> ]	1 × 10 <sup>4</sup>
$\text{TEMP}_{\text{test}}$	Temperature at which vapour pressure or water solubility was measured	[°C]	User input
$\text{SOL}(\text{TEMP}_{\text{env}})$	Solubility in water at environmental temperature (12 °C)	[mg.L <sup>-1</sup> ]	
$VP(\text{TEMP}_{\text{env}})$	Vapour Pressure at environmental temperature (12 °C)	[Pa]	

The concentration in porewater is calculated using Equation 43. As this concentration is used to calculate uptake by earthworms for the secondary poisoning assessment, the 180 day time weighted average PEC in soil has been used.

$$C_{\text{soil porewater}} = C_{\text{soil wwt}} \times RHO_{\text{soil}} / (K_{\text{soil-water}} \times 1000) \quad \text{Equation 43}$$

Explanation of symbols

$K_{\text{soil-water}}$	Soil-water partitioning coefficient	[mg.m <sup>-3</sup> ]	Equation 37
$RHO_{\text{soil}}$	Bulk density of wet soil	[kg.m <sup>-3</sup> ]	1700
$C_{\text{soil wwt}}$	Concentration in soil (wet weight) as a 180d time weighted average	[mg.kg <sub>wwt</sub> <sup>-1</sup> ]	Equation 35
$C_{\text{soil porewater}}$	Concentration in soil porewater	[mg.L <sup>-1</sup> ]	

### 3.6.3 Surface Water and Sediment model

The predicted environmental concentrations in surface water and sediment are calculated according to the Step 2 calculation approach developed by FOCUS (2003) for assessment of active ingredients in PPP. These FOCUS calculations are very conservative and provide an estimation of the potential loading of a substance to surface water via spray drift as well as entry into the waterbody due to heavy rainfall, triggering a runoff, erosion and/or drainage event.

Inputs of spray drift, runoff, erosion and/or drainage are evaluated as a series of individual loadings comprising of drift events followed by a loading representing a runoff, erosion and/or drainage event four days after the final application. Please note that the ‘Default’ assessment in the LET is conducted on a single application of the plant protection product, not multiple applications. Degradation is assumed to follow first-order kinetics in soil, surface water and sediment.

The LET adopts the standardised waterbody scenario used in FOCUS (2003) calculations, with 30 cm water depth overlying sediment of 5 cm depth. The sediment is assumed to have a density of 0.8 g/cm<sup>3</sup> and an organic carbon content of 5%. The waterbody is assumed to have an area equivalent to one tenth of the field from which it receives runoff or drainage water (a field: water ratio of 10). Assuming a 1 ha field, the 0.1 ha (1000 m<sup>2</sup>) waterbody will have a volume of 3 x 10<sup>5</sup> litres.

Daily concentrations in surface water and sediment are calculated. However, the PEC values reported in the LET are the maximum concentrations in surface water and sediment.

#### 3.6.3.1 Loadings to the waterbody

##### 3.6.3.1.1 Input into the waterbody via spray drift

The fraction of each application reaching the adjacent waterbody is dependent on formulation type, crop and the number of applications. The standard FOCUS Step 2 assumptions for spray drift are summarised in Table 26. For the LET ‘Default’ assessment, the spray drift value for one application to ‘fruit (late)’ was selected (see Table 21). This corresponds to a drift rate of 15.7% (this drift rate also applies to olives and citrus). It should be noted that some crops have higher drift rates than this. For example, ‘fruit (early)’ has a default drift rate of 29.2%. However, early applications are actually quite rare, since the trees have no foliage at that stage, so this was rejected for use as a realistic worst-case ‘Default’. The drift rate of 33.2% for aerial applications was also rejected as a realistic worst-case value, since applications of this type now require a derogation within the EU, and therefore cannot be considered to represent normal practice.

Crop type and the number of applications can be defined in the LET using the ‘Refinement Options’ assessment. Drift values are presented in Table 25 for twelve generic crop categories (these categories

also define the interception values). The use of these generic categories rather than specific crops is recommended if a higher-tier refinement of the exposure assessment is necessary.

**Table 25:** Spray-drift values for twelve generic crop categories

Crop	Distance crop- water (m)	% drift (Number of applications per season)								
		1	2	3	4	5	6	7	>7	
No drift (incorporation / seed treatment)	1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Vines, early applications	3	2.7	2.5	2.8	2.5	2.4	2.3	2.3	2.3	2.3
Hand applications (crop < 50 cm)	1	2.8	2.4	2.0	1.9	1.8	1.6	1.6	1.6	1.5
Spray to bare soil / pre-emergent use	1	2.8	2.4	2.0	1.9	1.8	1.6	1.6	1.6	1.5
Arable crops	1	2.8	2.4	2.0	1.9	1.8	1.6	1.6	1.6	1.5
Vegetable crops	1	2.8	2.4	2.0	1.9	1.8	1.6	1.6	1.6	1.5
Vines, late applications	3	8.0	7.1	6.9	6.6	6.6	6.4	6.2	6.2	6.2
Hand applications (crop > 50 cm)	3	8.0	7.1	6.9	6.6	6.6	6.4	6.2	6.2	6.2
Fruit (late)	3	15.7	12.1	11.0	10.1	9.7	9.2	9.1	8.7	8.7
Hops	3	19.3	17.7	15.9	15.4	15.1	14.9	14.6	13.5	13.5
Fruit (early)	3	29.2	15.5	24.0	23.6	23.1	22.8	22.7	22.2	22.2
Aerial application	3	33.2	33.2	33.2	33.2	33.2	33.2	33.2	33.2	33.2

To maintain transparency, the spray-drift values for a more detailed list of crops as used in FOCUS Step 2 are also implemented in the CLE LET (Table 26).

**Table 26:** FOCUS Step 2 crop spray-drift values aggregated according to % drift (FOCUS, 2003)

Crop	Distance crop- water (m)	% drift (Number of applications per season)								
		1	2	3	4	5	6	7	>7	
<b>Arable and vegetable crops:</b> (spring cereals, winter cereals, cotton, field beans, grass / alfalfa, legumes, maize, winter oil seed rape, spring oil seed rape, potatoes, soybeans, sugar beet, sunflower, tobacco, bulb vegetables, fruiting vegetables, leafy vegetables, root vegetables, application, hand (crop < 50 cm))	1	2.8	2.4	2.0	1.9	1.8	1.6	1.6	1.5	1.5
<b>Fruit (late)</b> Citrus, olives, pome / stone fruit (late)	3	15.7	12.1	11.0	10.1	9.7	9.2	9.1	8.7	8.7
<b>Fruit (early)</b> pome / stone fruit, (early)	3	29.2	25.5	24.0	23.6	23.1	22.8	22.7	22.2	22.2
<b>vines, early applications</b>	3	2.7	2.5	2.5	2.5	2.4	2.3	2.3	2.3	2.3
<b>vines, late applications</b>	3	8.0	7.1	6.9	6.6	6.6	6.4	6.2	6.2	6.2

Crop	Distance crop- water (m)	% drift (Number of applications per season)							
		1	2	3	4	5	6	7	>7
application, hand (crop > 50 cm)	3	8.0	7.1	6.9	6.6	6.6	6.4	6.2	6.2
hops	3	19.3	17.7	15.9	15.4	15.1	14.9	14.6	13.5
application, aerial	3	33.2	33.2	33.2	33.2	33.2	33.2	33.2	33.2
no drift (incorporation /seed treatment)	1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

The input into surface water via a single drift event is calculated as described in Equation 44.

$$\text{Input Drift} = \text{AR} \times \text{Drift \%} / 1000 \quad \text{Equation 44}$$

Explanation of symbols

<i>AR</i>	Equivalent application rate for co-formulant	[g.ha <sup>-1</sup> ]	User input
<i>Drift %</i>	Drift percentage	[%]	Table 26
<i>Input Drift</i>	Input via single drift event	[mg.m <sup>-2</sup> ]	

### 3.6.3.1.2 Input into the waterbody via runoff/drainage/erosion

The amount of substance available for runoff/drainage/erosion is dependent on the amount of co-formulant in the soil, region of application and the season of application. As in the FOCUS Step 2 model, the LET runoff/drainage/erosion event is driven by a rainfall event four days after the final application. Therefore, the amount of co-formulant present in the soil will be a function of formulation type, vapour pressure (if the substance is used for spray treatment), crop interception and degradation in soil until the rainfall event (4 days after the final treatment). The amount of co-formulant present in the soil after a single application is discussed in Section 3.6.2.4 and can be calculated using Equation 22.

The concentration in soil after the final application is calculated in Equation 45 and only includes biodegradation as a removal process (i.e., leaching and volatilisation are not included).

$$\text{Eq Rate Runoff Final} = \text{Soil loading} \times 1 - e^{(-N_{\text{app}} \times \text{App Int} \times \ln(2) / \text{DT}_{50\text{soil}})} / e^{(-\text{App Int} \times \ln(2) / \text{DT}_{50\text{soil}})} \quad \text{Equation 45}$$

Explanation of symbols

<i>DT<sub>50soil</sub></i>	Half-life of the co-formulant in soil	[days]	User input
<i>App Int</i>	Interval between applications	[days]	User input
<i>N<sub>app</sub></i>	Number of application events	[-]	User input
<i>Soil Loading</i>	Soil loading of the co-formulant	[g.ha <sup>-1</sup> ]	Equation 22
<i>Eq Rate Runoff Final</i>	Equivalent rate for runoff after the last treatment	[g.ha <sup>-1</sup> ]	

The rainfall event that drives the runoff/drainage/erosion event occurs 4 days after the last application and the equivalent application rate, 4 days after the final treatment, is calculated using Equation 46.

$$\text{Eq Rate Runoff Event} = \text{Eq Rate Runoff final} \times e^{(-4 \times \ln(2) / DT50_{\text{soil}})} \quad \text{Equation 46}$$

Explanation of symbols

$DT_{50\text{soil}}$	Half-life of the co-formulant in soil	[days]	User input
<i>Eq Rate Runoff Final</i>	Equivalent rate for runoff after the last treatment	[g.ha <sup>-1</sup> ]	Equation 45
<i>Eq Rate Runoff Event</i>	Equivalent rate for runoff at the time of the runoff event	[g.ha <sup>-1</sup> ]	

The fraction of co-formulant entering the waterbody at the runoff/drainage event is dependent on the region and season of application. The FOCUS Step 2 defaults for runoff are summarised in

Table 27. For the LET 'Default' assessment parameterisation, the worst-case runoff value of 5% for 'North Europe, Oct – Feb' has been assumed (see Table 21), giving a worst-case assessment of exposure via runoff. The region and season of application can be defined by selecting 'Refinement option'.

**Table 27:** Input into waterbody via runoff/drainage (FOCUS, 2003)

Region/season	% of soil residue moved to waterbody (Runoff %)
North Europe, Oct. - Feb.	5
North Europe, Mar. – May	2
North Europe, June - Sep.	2
South Europe, Oct. - Feb.	4
South Europe, Mar. - May	4
South Europe, June - Sep.	3
No Runoff	0

The input to the waterbody via runoff can be calculated as shown in Equation 47 where the waterbody is assumed to have an area equivalent to one tenth of the field from which it receives runoff or drainage water.

$$\text{Input Runoff} = \text{Eq Rate Runoff Event} \times \text{Runoff \%} \times \text{FW Ratio} / 1000 \quad \text{Equation 47}$$

Explanation of symbols

<i>Eq Rate Runoff Event</i>	Equivalent rate for runoff at the time of the runoff event	[g.ha <sup>-1</sup> ]	Equation 46
<i>Runoff %</i>	Runoff percentage (related to soil residue)	[%]	Default: 5% Refinement: Table 27
<i>FW Ratio</i>	Ratio of field to waterbody	[-]	10

<i>Input Runoff</i>	Input via runoff	[mg.m <sup>-2</sup> ]
---------------------	------------------	-----------------------

Equation 47 calculates the amount of co-formulant that will be inputted into the waterbody via runoff/drainage/erosion following a rainfall event. However, the fraction of co-formulant entering the waterbody in the water phase and in the sediment phase will be dependent on the soil adsorption ( $K_{OC}$ ) of the substance.

### 3.6.3.1.3 Input to waterbody in water and sediment phase via runoff/drainage/erosion

The fraction entering the waterbody in the water phase via runoff/drainage/erosion is calculated according to the soil adsorption ( $K_{OC}$ ) of the substance (Equation 48).

$$F_{\text{water phase runoff}} = \text{Water Depth} / (\text{Water Depth} + \text{Eff Sed Depth} \times \text{RHOSed} \times \text{OC} \times K_{oc} / 100) \quad \text{Equation 48}$$

Explanation of symbols

<i>Water Depth</i>	Depth of the surface water	[cm]	30
<i>Eff Sed Depth</i>	Effective sediment depth of the surface water	[cm]	1
<i>RHOSed</i>	Sediment bulk density	[kg.L <sup>-1</sup> ]	0.8
<i>OC</i>	Sediment organic carbon content	[%]	5
<i>Koc</i>	Soil sorption constant related to org carbon	[L.kg <sup>-1</sup> ]	User input
<i>Fwater phase runoff</i>	Fraction of substance entering in water phase via runoff	[-]	

The total loading to the waterbody, entering in the water phase and sediment phase are calculated according to Equation 49 and Equation 50, respectively.

$$\text{Input Runoff}_{\text{sw}} = \text{Input Runoff} \times F_{\text{water phase runoff}} \quad \text{Equation 49}$$

$$\text{Input Runoff}_{\text{sed}} = \text{Input Runoff} \times (1 - F_{\text{water phase runoff}}) \quad \text{Equation 50}$$

Explanation of symbols

<i>Fwater phase runoff</i>	Fraction of substance entering in water phase via runoff	[-]	Equation 48
<i>Input Runoff</i>	Total input via runoff	[mg.m <sup>-2</sup> ]	Equation 47
<i>Input Runoff<sub>sw</sub></i>	Runoff input via water phase	[mg.m <sup>-2</sup> ]	
<i>Input Runoff<sub>sed</sub></i>	Runoff input via sediment phase	[mg.m <sup>-2</sup> ]	

### 3.6.3.2 Calculation of daily concentrations

In the LET, as for FOCUS Step 2, the loadings into the waterbody occur as a series of individual applications with drift to the waterbody, followed by a runoff/erosion/drainage event occurring four days after the last application. The drift input fully enters the surface water without any distribution, whereas the input via runoff/drainage is immediately distributed between the water and sediment layer. After the occurrence of the runoff/drainage event it is assumed that full equilibrium between water and sediment is established within 24 hours.

$$\text{Input}_{\text{sw}}(\text{app}) = \text{Input Drift} \quad \text{Equation 51}$$

$$\text{Input}_{\text{sed}}(\text{app}) = 0 \quad \text{Equation 52}$$

Explanation of symbols

<i>Input Drift</i>	Input via a single drift event	[mg.m <sup>-2</sup> ]	Equation 44
<i>Input<sub>sw</sub>(app)</i>	Input into the water phase, on the day of application	[mg.m <sup>-2</sup> ]	
<i>Input<sub>sed</sub>(app)</i>	Input into the sediment phase, on the day of application	[mg.m <sup>-2</sup> ]	

$$\text{Input}_{\text{sw}}(\text{storm}) = \text{Input Runoff}_{\text{sw}} \quad \text{Equation 53}$$

$$\text{Input}_{\text{sed}}(\text{storm}) = \text{Input Runoff}_{\text{sed}} \quad \text{Equation 54}$$

Explanation of symbols

<i>Input Runoff<sub>sw</sub></i>	Runoff input via water phase	[mg.m <sup>-2</sup> ]	Equation 49
<i>Input Runoff<sub>sed</sub></i>	Runoff input via sediment phase	[mg.m <sup>-2</sup> ]	Equation 50
<i>Input<sub>sw</sub>(storm)</i>	Input into the water phase, on the day of erosion/drainage/runoff event	[mg.m <sup>-2</sup> ]	
<i>Input<sub>sed</sub>(storm)</i>	Input into the sediment phase, on the day of erosion/drainage/runoff event	[mg.m <sup>-2</sup> ]	

### 3.6.3.2.1 On Day 0

On the first simulation day, the input via a single drift event is taken to calculate the substance mass in the water phase. No input is considered for the sediment phase.

$$\text{Mass}_{\text{sw}}(0) = \text{Input}_{\text{sw}}(\text{app}) = \text{Input Drift} \quad \text{Equation 55}$$

$$\text{Mass}_{\text{sed}}(0) = \text{Input}_{\text{sed}}(\text{app}) = 0 \quad \text{Equation 56}$$

Explanation of symbols

<i>Input Drift</i>	Input via single drift event	[mg.m <sup>-2</sup> ]	Equation 44
<i>Input<sub>sw</sub>(app)</i>	Input into the water phase, on the day of application	[mg.m <sup>-2</sup> ]	
<i>Input<sub>sed</sub>(app)</i>	Input into the sediment phase, on the day of application	[mg.m <sup>-2</sup> ]	
<i>Mass<sub>sw</sub>(0)</i>	Substance mass in the surface water on day 0	[mg.m <sup>-2</sup> ]	
<i>Mass<sub>sed</sub>(0)</i>	Substance mass in the sediment on day 0	[mg.m <sup>-2</sup> ]	

At the end of day 0 (just before day 1) the distribution of the substance between the water and sediment layer is calculated for the first time (without considering degradation). It is assumed (as in FOCUS Step 2) that the substance is distributed in surface water into two theoretical compartments, one “available” for sorption to sediment and the other “unavailable” for sorption to sediment. The fractions available



for sorption and unavailable for sorption in surface water are calculated in Equation 57 and Equation 58.

$$\text{Mass}_{\text{swintavailable}}(0) = \text{Mass}_{\text{swint}}(0) / \text{Dist Coeff} \quad \text{Equation 57}$$

$$\text{Mass}_{\text{swintunavailable}}(0) = \text{Mass}_{\text{swint}}(0) - \text{Mass}_{\text{swintavailable}}(0) \quad \text{Equation 58}$$

#### Explanation of symbols

$\text{Mass}_{\text{swint}}(0)$	Temporary substance mass in the surface water at the end of day 0	[mg.m <sup>-2</sup> ]	Equation 55
<i>Dist Coeff</i>	Distribution coefficient	[-]	1.5 (on day 0)
$\text{Mass}_{\text{swintavailable}}(0)$	Temporary substance mass in the surface water at the end of day 0 that is available for sorption	[mg.m <sup>-2</sup> ]	
$\text{Mass}_{\text{swintunavailable}}(0)$	Temporary substance mass in the surface water at the end of day 0 that is not available for sorption	[mg.m <sup>-2</sup> ]	

The mass distribution between water and sediment at the end of day 0 is then estimated based on the intermediate results.

$$\text{Mass}_{\text{sw}}(\text{end\_day\_0}) = \text{Mass}_{\text{swintunavailable}}(0) + (\text{Mass}_{\text{swintavailable}}(0) + \text{Mass}_{\text{sedint}}(0)) \times \text{Fwaterphase}_{\text{runoff}} \quad \text{Equation 59}$$

$$\text{Mass}_{\text{sed}}(\text{end\_day\_0}) = \text{Mass}_{\text{swint}}(0) + \text{Mass}_{\text{sedint}}(0) - \text{Mass}_{\text{sw}}(\text{end\_day\_0}) \quad \text{Equation 60}$$

#### Explanation of symbols

$\text{Mass}_{\text{swint}}(0)$	Temporary substance mass in the surface water at the end of day 0	[mg.m <sup>-2</sup> ]	Equation 55
$\text{Mass}_{\text{sedint}}(0)$	Temporary substance mass in the sediment at the end of day 0	[mg.m <sup>-2</sup> ]	Equation 56
<i>Fwater phase<sub>runoff</sub></i>	Fraction of compound entering in water phase <i>via</i> runoff	[-]	Equation 48
$\text{Mass}_{\text{swintavailable}}(0)$	Temporary substance mass in the surface water at the end of day 0 that is available for sorption	[mg.m <sup>-2</sup> ]	Equation 57
$\text{Mass}_{\text{swintunavailable}}(0)$	Temporary substance mass in the surface water at the end of day 0 that is not available for sorption	[mg.m <sup>-2</sup> ]	Equation 58
$\text{Mass}_{\text{sw}}(\text{end\_day\_0})$	Substance mass in the surface water at the end of day 0	[mg.m <sup>-2</sup> ]	
$\text{Mass}_{\text{sed}}(\text{end\_day\_0})$	Substance mass in the sediment at the end of day 0	[mg.m <sup>-2</sup> ]	

#### 3.6.3.2.2 On Day *i* (>0)

The daily concentrations for the following simulation days are calculated using a stepwise approach based on the current substance masses in the compartments. First, a temporary mass of the substance in water and sediment is calculated considering degradation of the amount remaining from the previous day and input from drift and runoff/drainage events.

$$\text{Mass}_{\text{swint}}(i) = \text{Mass}_{\text{sw}}(i-1) \times e^{(-\ln(2) / DT_{50_{\text{sw}}})} + \text{Input}_{\text{sw}}(i) \quad \text{Equation 61}$$

$$\text{Mass}_{\text{sedint}}(i) = \text{Mass}_{\text{sed}}(i-1) \times e^{(-\ln(2) / DT_{50_{\text{sed}}})} + \text{Input}_{\text{sed}}(i) \quad \text{Equation 62}$$

## Explanation of symbols

$\text{Mass}_{\text{sw}}(i-1)$	Substance mass in the surface water on day i-1	[mg.m <sup>-2</sup> ]	If i= 1 then: Equation 59 Otherwise: Equation 65
$\text{Mass}_{\text{sed}}(i-1)$	Substance mass in the sediment on day i-1	[mg.m <sup>-2</sup> ]	If i= 1 then: Equation 60 Otherwise: Equation 66
$\text{Input}_{\text{sw}}(i)$	Input into the water phase, on day i	[mg.m <sup>-2</sup> ]	Equation 44 and Equation 53
$\text{Input}_{\text{sed}}(i)$	Input into the sediment phase, on day i	[mg.m <sup>-2</sup> ]	Equation 54
$DT_{50_{\text{sw}}}$	Half-life of the substance in surface water	[days]	User input
$DT_{50_{\text{sed}}}$	Half-life of the substance in sediment	[days]	User input
$\text{Mass}_{\text{swint}}(i)$	Temporary substance mass in the surface water on day i	[mg.m <sup>-2</sup> ]	
$\text{Mass}_{\text{sedint}}(i)$	Temporary substance mass in the sediment on day i	[mg.m <sup>-2</sup> ]	

The fraction of substance that enters the waterbody *via* drift on day *i* is assumed to be partitioned between water and sediment in the following days. As in day 0, the substance is distributed in surface water into two theoretical compartments, “available” for sorption to sediment and “unavailable” for sorption to sediment.

$$\text{Mass}_{\text{swintavailable}}(i) = \text{Mass}_{\text{swint}}(i) / \text{Dist Coeff} \quad \text{Equation 63}$$

$$\text{Mass}_{\text{swintunavailable}}(i) = \text{Mass}_{\text{swint}}(i) - \text{Mass}_{\text{swintavailable}}(i) \quad \text{Equation 64}$$

## Explanation of symbols

$\text{Mass}_{\text{swint}}(i)$	Temporary substance mass in the surface water on day <i>i</i>	[mg.m <sup>-2</sup> ]	Equation 61
$\text{Dist Coeff}$	Distribution coefficient	[-]	Before the runoff event = 1.5 During and after the runoff event = 1
$\text{Mass}_{\text{swintavailable}}(i)$	Temporary substance mass in the surface water on day <i>i</i> that is available for sorption	[mg.m <sup>-2</sup> ]	
$\text{Mass}_{\text{swintunavailable}}(i)$	Temporary substance mass in the surface water on day <i>i</i> that is not available for sorption	[mg.m <sup>-2</sup> ]	

The distribution of the substance in surface water and sediment on day *i* is calculated according to the substance fraction in water available for sorption:

$$\text{Mass}_{\text{sw}}(i) = \text{Mass}_{\text{swintunavailable}}(i) + (\text{Mass}_{\text{swinavailable}}(i) + \text{Mass}_{\text{sedint}}(i) \times \text{Fwaterphase}_{\text{runoff}})$$
 Equation 65

$$\text{Mass}_{\text{sed}}(i) = \text{Mass}_{\text{swint}}(i) + \text{Mass}_{\text{sedint}}(i) - \text{Mass}_{\text{sw}}(i)$$
 Equation 66

## Explanation of symbols

$\text{Mass}_{\text{swint}}(i)$	Temporary substance mass in the surface water on day $i$	[mg.m <sup>-2</sup> ]	Equation 61
$\text{Mass}_{\text{sedint}}(i)$	Temporary substance mass in the sediment on day $i$	[mg.m <sup>-2</sup> ]	Equation 62
$\text{Fwater phase}_{\text{runoff}}$	Fraction of substance entering in water phase via runoff	[-]	Equation 48
$\text{Mass}_{\text{swintavailable}}(i)$	Temporary substance mass in the surface water on day $i$ that is available for sorption	[mg.m <sup>-2</sup> ]	Equation 63
$\text{Mass}_{\text{swintunavailable}}(i)$	Temporary substance mass in the surface water on day $i$ that is not available for sorption	[mg.m <sup>-2</sup> ]	Equation 64
$\text{Mass}_{\text{sw}}(i)$	Substance mass in the surface water on day $i$	[mg.m <sup>-2</sup> ]	
$\text{Mass}_{\text{sed}}(i)$	Substance mass in the sediment on day $i$	[mg.m <sup>-2</sup> ]	

## 3.6.3.2.3 Local concentration in surface water and sediment

As with FOCUS Step 2, the local concentrations in surface water and sediment are reported as daily concentrations based on the masses in the system before the distribution between water and sediment is considered.

$$\text{Clocal}_{\text{sw}}(i) = \text{Mass}_{\text{swint}}(i) \times 100 / \text{Water Depth}$$
 Equation 67

$$\text{Clocal}_{\text{sed}}(i) = \text{Mass}_{\text{sedint}}(i) \times / (\text{Sed Depth} \times \text{RHOSed})$$
 Equation 68

## Explanation of symbols

$\text{Mass}_{\text{swint}}(i)$	Temporary substance mass in the surface water on day $i$	[mg.m <sup>-2</sup> ]	Equation 61
$\text{Mass}_{\text{sedint}}(i)$	Temporary substance mass in the sediment on day $i$	[mg.m <sup>-2</sup> ]	Equation 62
$\text{Water Depth}$	Depth of the surface water	[cm]	30
$\text{Sed Depth}$	Sediment depth	[cm]	5
$\text{RHOSed}$	Sediment bulk density	[kg.L <sup>-1</sup> ]	0.8
$\text{Clocal}_{\text{sw}}(i)$	Surface water concentration on day $i$	[µg.L <sup>-1</sup> ]	
$\text{Clocal}_{\text{SED}}(i)$	Sediment concentration on day $i$	[µg.kg <sub>dwt</sub> <sup>-1</sup> ]	

Daily local concentrations in surface water and sediment are calculated using Equation 67 and Equation 68, respectively. The maximum local concentrations in surface water and sediment are calculated using Equation 69 and Equation 70, respectively, and then used in the risk characterisation ratios for surface water and sediment (see Section 3.6.6).

$$C_{local_{sw}} = \text{Maximum } C_{local_{sw}(i)} \quad \text{Equation 69}$$

Explanation of symbols

$C_{local_{sw}(i)}$	Surface water concentration on day $i$	$[\mu\text{g}\cdot\text{L}^{-1}]$	Equation 67
$C_{local_{sw}}$	Maximum local freshwater concentration	$[\mu\text{g}\cdot\text{L}^{-1}]$	

$$C_{local_{sed}(dwt)} = \text{Maximum } C_{local_{sed}(i)} \quad \text{Equation 70}$$

Explanation of symbols

$C_{local_{SED}(i)}$	Sediment concentration on day $i$	$[\mu\text{g}\cdot\text{kg}_{dwt}^{-1}]$	Equation 68
$C_{local_{sed}(dwt)}$	Maximum local freshwater sediment concentration (dry weight)	$[\mu\text{g}\cdot\text{kg}_{dwt}^{-1}]$	

#### 3.6.3.2.4 Local concentration in marine water and marine water sediment

The local concentrations for marine water and marine water sediment are calculated for situations where there may be specific release into the marine environment. This would be expected where an industrial site is located on the coast or where a substance is used in the catchment of a coastal sewage treatment plant (STP), which releases directly into the marine environment. Use of a co-formulant adjacent to a coastal waterbody is extremely unlikely; nevertheless, the LET calculates local concentrations for marine water and marine-water sediment in accordance with the REACH requirement for a local-scale exposure assessment. As a conservative assumption a dilution factor of 10 has been applied to the local concentrations in surface water and sediment calculated in Equation 69 and Equation 70. While this does not account for possible differences in partitioning behaviour in the marine environment, a dilution factor of 10 is a conservative assumption. It is expected that local concentrations for marine water and marine water sediment calculated in Equation 71 and Equation 72 will be worst-case.

$$C_{local_{marine\ water}} = C_{local_{sw}} / 10 \quad \text{Equation 71}$$

$$C_{local_{marine\ sed\ (dwt)}} = C_{local_{sed\ (dwt)}} / 10 \quad \text{Equation 72}$$

Explanation of symbols

$C_{local_{sw}}$	Maximum local freshwater concentration	$[\mu\text{g}\cdot\text{L}^{-1}]$	Equation 69
$C_{local_{sed}(dwt)}$	Maximum local freshwater sediment concentration (dry weight)	$[\text{mg}\cdot\text{kg}_{dwt}^{-1}]$	Equation 70
$C_{local_{marine\ water}}$	Local marine water concentration	$[\mu\text{g}\cdot\text{L}^{-1}]$	
$C_{local_{marine\ sed\ (dwt)}}$	Local marine sediment concentration (dry weight)	$[\text{mg}\cdot\text{kg}_{dwt}^{-1}]$	

#### 3.6.3.2.5 Time-weighted average concentration in surface water and sediment

The first step to calculating the time weighted average concentrations is to calculate the 1 day averaged concentrations in surface water and sediment using Equation 73 and Equation 74.

$$C_{local\_24TWA_{sw}(i)} = (C_{local_{sw}(i-1)} + C_{local_{sw}(i)}) / 2 \quad \text{Equation 73}$$

$$C_{local\_24TWA_{sed}(i)} = (C_{local_{sed}(i-1)} + C_{local_{sed}(i)}) / 2 \quad \text{Equation 74}$$

## Explanation of symbols

$Clocal_{SW}(i-1)$	Surface water concentration on day $i-1$	$[\mu\text{g}\cdot\text{L}^{-1}]$	Equation 67
$Clocal_{SED}(i-1)$	Sediment concentration on day $i-1$	$[\mu\text{g}\cdot\text{kg}_{\text{dwt}}^{-1}]$	Equation 68
$Clocal_{SW}(i)$	Surface water concentration on day $i$	$[\mu\text{g}\cdot\text{L}^{-1}]$	Equation 67
$Clocal_{SED}(i)$	Sediment concentration on day $i$	$[\mu\text{g}\cdot\text{kg}_{\text{dwt}}^{-1}]$	Equation 68
$Clocal_{24TWA_{SW}}(i)$	24 hour averaged surface water concentration on day $i$	$[\mu\text{g}\cdot\text{L}^{-1}]$	
$Clocal_{24TWA_{SED}}(i)$	24 hour averaged sediment concentration on day $i$	$[\mu\text{g}\cdot\text{kg}_{\text{dwt}}^{-1}]$	

The time weighted average concentrations in surface water and sediment are calculated from the maximum local concentrations in surface water and sediment over time period,  $t$ , as defined as:

$$TWAC_{\text{sw}}(t) = \sum_{i=i_{\text{max}}+1}^{i_{\text{max}}+t} Clocal_{24TWA_{\text{sw}}}(i) / t \quad \text{Equation 75}$$

$$TWAC_{\text{sed}}(t) = \sum_{i=i_{\text{max}}+1}^{i_{\text{max}}+t} Clocal_{24TWA_{\text{sed}}}(i) / t \quad \text{Equation 76}$$

## Explanation of symbols

$Clocal_{24TWA_{SW}}(i)$	24 hour averaged surface water concentration on day $i$	$[\mu\text{g}\cdot\text{L}^{-1}]$	Equation 73
$Clocal_{24TWA_{SED}}(i)$	24 hour averaged sediment concentration on day $i$	$[\mu\text{g}\cdot\text{kg}_{\text{dwt}}^{-1}]$	Equation 74
$i_{\text{max}}$	Day of the maximum surface water or sediment concentration	[d]	
$t$	Time period	[d]	Secondary poisoning: 21 Humans via environment: 21
$TWAC_{\text{sw}}(t)$	Time weighted average concentration in surface water, over a period $t$	$[\mu\text{g}\cdot\text{L}^{-1}]$	
$TWAC_{\text{SED}}(t)$	Time weighted average concentration in sediment, over a period $t$	$[\mu\text{g}\cdot\text{kg}_{\text{dwt}}^{-1}]$	

The local concentration in surface water used for the aquatic secondary poisoning assessment is the 21-day time weighted average surface water concentration in accordance with the approach used in the assessment of PPP. This deviates slightly from the EU-TGD (2003) and ECHA R.16 guidance (2016) which assumes the annual average concentration in surface water (see Section 3.6.4.2.1.1). The local surface water concentration used to calculate the PEC in fish for human consumption is also the 21 day time weighted average and this is calculated using Equation 78.

$$Clocal_{\text{sw,secondary poisoning}} = TWAC_{\text{sw}}(21\text{d}) \quad \text{Equation 77}$$

$$Clocal_{\text{sw,HvE, fish}} = TWAC_{\text{sw}}(21\text{d}) \quad \text{Equation 78}$$

The corresponding local marine water concentration used for the marine water secondary poisoning assessment is calculated using Equation 79.

$$\text{Clocal}_{\text{mw,secondary poisoning}} = \text{Clocal}_{\text{sw}(21\text{d})} / 10$$

Equation 79

### 3.6.4 Secondary poisoning model

According to the ECHA guidance R.16 (2016, Section R.16.1.3.2), a detailed assessment of secondary poisoning should be conducted if there are indications for bioaccumulation potential, low degradability (e.g., not readily biodegradable or not hydrolysable) and the substance has the potential to cause toxic effects if accumulated in higher organisms.

The screening criteria for indications of bioaccumulation potential according to R.16.1.3.2 are:

- the substance has a  $\log K_{\text{OW}} \geq 3$  and a molecular weight below 700 g/mol; or;
- is highly adsorptive; or;
- belongs to a class of substances known to have a potential to accumulate in living organisms; or;
- there are indications from structural features;
- and there are no mitigating properties (e.g., hydrolysis).

The screening criteria for indications of a potential toxic effect in higher organisms according to R.16.1.3.2 are:

- The available mammalian toxicity data can give an indication on the possible risks of the substance to higher organisms in the environment.
- This assessment is based on classifications on the basis of mammalian toxicity data, i.e., the classification includes one of the hazard statements:
  - H360 “May damage fertility or the unborn child”,
  - H361 “Suspected of damaging fertility or the unborn child”,
  - H362 “May cause harm to breastfed children”,
  - H372 “Causes damage to organs through prolonged or repeated exposure”,
  - H373 “May cause damage to organs through prolonged or repeated exposure”.
- When available, avian toxicity may also be taken into account.

The LET allows an assessment of secondary poisoning of terrestrial predators (earthworm eating), aquatic predators (fish eating and marine fish eating) and marine top predators to be conducted, using the equations from the ECHA R.16 guidance (2016) and the EU-TGD (2003).

#### 3.6.4.1 Secondary poisoning via the aquatic food chain

##### 3.6.4.1.1 Bioconcentration and biomagnification in the aquatic environment

The bioconcentration factor (BCF) and the biomagnification factor (BMF) for fish are used to estimate the concentration of a contaminant in the food (fish) of fish-eating predators. Where a measured BCF value is available, this is used directly in Equation 82 to Equation 89. If experimental data are not available, the BCF for fish can be predicted from the relationship between  $K_{\text{OW}}$  and BCF derived by Veith *et al.*, (1979). For substances with a  $\log K_{\text{OW}}$  of 2 to 6, the BCF in fish is estimated using Equation 80.

$$\log \text{BCF}_{\text{fish}} = 0.85 \times \log K_{\text{OW}} - 0.70$$

Equation 80

For substances with a  $\log K_{\text{OW}}$  higher than 6, Equation 81 is used:

$$\log BCF_{\text{fish}} = -0.20 \times \log K_{\text{ow}}^2 + 2.74 \times \log K_{\text{ow}} - 4.72 \quad \text{Equation 81}$$

## Explanation of symbols

$K_{\text{ow}}$	Octanol-water partition coefficient	[-]	User input
$BCF_{\text{fish}}$	Bioconcentration factor for fish on wet weight basis	[L.kg <sub>wet fish</sub> <sup>-1</sup> ]	

This approach is considered appropriate to estimate  $BCF_{\text{fish}}$  when the  $\log K_{\text{ow}}$  is between 1 and 10. If the  $\log K_{\text{ow}}$  is outside this range, other approaches may need to be considered. It is recommended to consult the ECHA endpoint-specific guidance R.7c in these cases.

The  $BMF_1$  in fish is also determined from the measured  $BCF$  (if available) or  $K_{\text{ow}}$  with default  $BMF_1$  values summarised in Table 28. Exposure of marine top predators can be the result of very hydrophobic substances biomagnifying in the tissues and organs of predators. To account for this an additional biomagnification factor ( $BMF_2$ ) is applied to the concentration in predators (Table 28). When measured  $BCF$  values are available, these are used to determine the  $BMF$  values.

**Table 28:** Default  $BMF$  values for organic substances (ECHA R16 guidance R.16.5.3.5, (2016))

log $K_{\text{ow}}$ of substance	BCF (fish)	$BMF_1$	$BMF_2$
<4.5	<2,000	1	1
4.5 - <5	2,000 – 5000	2	2
5 – 8	>5,000	10	10
>8 – 9	2,000 – 5,000	3	3
>9	<2,000	1	1

### 3.6.4.2 PEC secondary poisoning (Aquatic Food Chain)

#### 3.6.4.2.1.1 Freshwater environment

The  $PEC$  in the food of the freshwater aquatic predator is calculated from the 21-day time weighted average  $PEC_{\text{surface water}}$ , bioconcentration in fish and the biomagnification factor (Equation 82). This is the standard approach in the assessment of active substances in PPP.

$$PEC_{\text{oral,predator}} = PEC_{\text{sw}} \times BCF_{\text{fish}} \times BMF_1 \quad \text{Equation 82}$$

Where:

$$PEC_{\text{sw}} = C_{\text{local,secondary poisoning}} / 1000 + PEC_{\text{regional,sw(dissolved)}} \quad \text{Equation 83}$$

## Explanation of symbols

$PEC_{\text{sw}}$	PEC in surface water at local scale	[mg.L <sup>-1</sup> ]	
$C_{\text{local,secondary poisoning}}$	21-day TWA surface water concentration	[µg.L <sup>-1</sup> ]	Equation 77
$PEC_{\text{regional,sw(dissolved)}}$	Surface water concentration at the regional scale (dissolved)	[mg.L <sup>-1</sup> ]	Input (calculated outside LET) otherwise assumed to be 0

$BCF_{fish}$	Bioconcentration factor for fish on wet weight basis	$[L.kg_{wet\ fish}^{-1}]$	Measured or estimated from $\log K_{ow}$ (Equation 80 and Equation 81)
$BMF_1$	Biomagnification factor in fish	[-]	Table 28
$PEC_{oral, predator}$	Predicted environmental concentration in food	$[mg.kg_{wet\ fish}^{-1}]$	

In the LET, the PEC in surface water used for the aquatic secondary poisoning assessment is the sum of the 21-day time weighted average surface water concentration (in accordance with the approach used in the assessment of PPP) and the regional concentration in surface water (where the regional concentration is assumed to be the background concentration for the local scale). This is a conservative, worst-case approach as it assumes the diet of the aquatic predator is continually exposed to the 21-day TWA PEC in surface water. This deviates slightly from the EU-TGD (2003) and ECHA R.16 guidance (2016) which assumes the annual average concentration in surface water rather than the 21-day TWA surface water concentration is used in the assessment.

Equation 82 reflects a situation where the aquatic (fish eating) predator consumes 100% of its diet from the local environment (in a waterbody adjacent to a treated field). In reality this is unlikely as the foraging area of the freshwater aquatic predator is expected to be larger than an edge of field waterbody.

Where regional PECs in surface water are available, it is assumed that 50% of a predator's diet comes from the local scale and 50% is assumed to come from the regional area (Equation 84).

$$PEC_{oral, predator} = 0.5 \times (PEC_{sw} + PEC_{regional_{sw(dissolved)}}) \times BCF_{fish} \times BMF \quad \text{Equation 84}$$

#### 3.6.4.2.1.2 Marine water environment

The PEC in the food of the marine water aquatic predator is calculated from the 21-day time-weighted average  $PEC_{marine\ water}$ , bioconcentration in fish and the biomagnification factor (Equation 85), in analogy to the approach used for the freshwater environment.

$$PEC_{oral, marine predator} = PEC_{mw} \times BCF_{fish} \times BMF_1 \quad \text{Equation 85}$$

Where:

$$PEC_{mw} = C_{local_{mw, secondary poisoning}} / 1000 + PEC_{regional_{mw(dissolved)}} \quad \text{Equation 86}$$

#### Explanation of symbols

$PEC_{mw}$	PEC in marine water at local scale	$[mg.L^{-1}]$	
$C_{local_{mw, secondary poisoning}}$	21-day TWA marine water concentration	$[\mu g.L^{-1}]$	Equation 79
$PEC_{regional_{mw(dissolved)}}$	Marine water concentration at the regional scale (dissolved)	$[mg.L^{-1}]$	Input (calculated outside LET) otherwise assumed to be 0
$BCF_{fish}$	Bioconcentration factor for fish on wet weight basis	$[L.kg_{wet\ fish}^{-1}]$	Measured or estimated from $\log K_{ow}$ (Equation 80 and Equation 81)



			80 and Equation 81)
$BMF_1$	Biomagnification factor in fish	[-]	Table 28
$PEC_{oral, marine predator}$	Predicted environmental concentration in food	$[mg.kg_{wet fish}^{-1}]$	

Equation 86 reflects a situation where the marine (fish eating) predator consumes 100% of its diet from the local environment (in coastal water adjacent to a treated field). In reality this is unlikely as the foraging area of the marine water aquatic predator is expected to be larger.

Where regional PECs in marine water are available, it is assumed that 50% of a predator's diet comes from the local scale and 50% is assumed to come from the regional area (Equation 87).

$$PEC_{oral, marine predator} = 0.5 \times (PEC_{mw} + PEC_{regional, mw(dissolved)}) \times BCF_{fish} \times BMF_1 \quad \text{Equation 87}$$

The PEC in the food of the top predator is calculated from the 21-day TWA  $PEC_{marine water}$ , bioconcentration in fish and biomagnification factors (Equation 88).

$$PEC_{oral, top predator} = PEC_{mw} \times BCF_{fish} \times BMF_1 \times BMF_2 \quad \text{Equation 88}$$

#### Explanation of symbols

$PEC_{mw}$	21-day TWA PEC in marine water at local scale	$[mg.L^{-1}]$	Equation 86
$BCF_{fish}$	Bioconcentration factor for fish on wet weight basis	$[L.kg_{wet fish}^{-1}]$	Measured or estimated from $\log K_{ow}$ (Equation 80 and Equation 81)
$BMF_1$	Biomagnification factor in fish	[-]	Table 28
$BMF_2$	Biomagnification factor in predator	[-]	Table 28
$PEC_{oral, marine predator}$	Predicted environmental concentration in food	$[mg.kg_{wet fish}^{-1}]$	

It is assumed for top predators that they mainly prey on organisms from the regional marine environment rather than the local scale. Therefore, where regional PECs in marine water are available, it is assumed that 10% of a top predator's diet comes from the local scale and 90% is assumed to come from the regional area (Equation 89).

$$PEC_{oral, top predator} = (0.1 \times PEC_{mw} + 0.9 \times PEC_{regional, mw(dissolved)}) \times BCF_{fish} \times BMF_1 \times BMF_2 \quad \text{Equation 89}$$

### 3.6.4.3 Secondary poisoning via the terrestrial food chain

#### 3.6.4.3.1 Bioconcentration in the terrestrial environment

For many organic chemicals, the main route of uptake into earthworms will be *via* the interstitial water. Where a measured bioconcentration factor (BCF) is available, this is used directly in Equation 91 and Equation 95. If experimental data are not available, bioconcentration in earthworms can be estimated according to Equation 90 described by Jager (1998).

$$BCF_{\text{earthworm}} = (0.84 + 0.012 \times K_{ow}) / RHO_{\text{earthworm}} \quad \text{Equation 90}$$

#### Explanation of symbols

$RHO_{\text{earthworm}}$	Earthworm density	[kg <sub>wwt</sub> .L <sup>-1</sup> ]	1
$K_{ow}$	Octanol-water partition coefficient	[-]	User input
$BCF_{\text{earthworm}}$	Bioconcentration factor for earthworms on wet weight basis	[L.kg <sub>wet earthworm</sub> <sup>-1</sup> ]	

#### 3.6.4.3.2 PEC secondary poisoning (Terrestrial Food Chain)

The predicted environmental concentration in food for terrestrial predators is equal to the concentration in the earthworm as a result of bioaccumulation in worm tissues and adsorption of the substance to soil present in the gut. The  $PEC_{\text{oral predator}}$  is calculated using Equation 91.

$$PEC_{\text{oral predator}} = C_{\text{earthworm}} = (BCF_{\text{earthworm}} \times PEC_{\text{porewater, sec. poisoning}} + PEC_{\text{soil, sec. poisoning}} \times F_{\text{gut}} \times CONV_{\text{soil}}) / (1 + F_{\text{gut}} \times CONV_{\text{soil}})$$

Equation 91

Where:

$$CONV_{\text{soil}} = RHO_{\text{soil}} / (F_{\text{solid}} \times RHO_{\text{solid}}) \quad \text{Equation 92}$$

$$PEC_{\text{porewater, sec. poisoning}} = C_{\text{soil porewater}} + PEC_{\text{regional agric. soil}} \times RHO_{\text{soil}} / (K_{\text{soil-water}} \times 1000) \quad \text{Equation 93}$$

$$PEC_{\text{soil, sec. poisoning}} = TWAC_{\text{soil}(180d)} + PEC_{\text{regional agric. soil}} \quad \text{Equation 94}$$

#### Explanation of symbols

$BCF_{\text{earthworm}}$	Bioconcentration factor for earthworms on wet weight basis	[L.kg <sub>wet earthworm</sub> <sup>-1</sup> ]	Measured or estimated from log $K_{ow}$ (Equation 90)
$PEC_{\text{porewater, sec. poisoning}}$	Predicted environmental concentration in porewater at local scale for secondary poisoning	[mg.L <sup>-1</sup> ]	Equation 93
$PEC_{\text{soil, sec. poisoning}}$	Predicted environmental concentration in soil at local scale for secondary poisoning	[mg.kg <sub>wwt</sub> <sup>-1</sup> ]	Equation 94
$F_{\text{gut}}$	Fraction of gut loading in worm	[kg <sub>dwt</sub> .kg <sub>wwt</sub> <sup>-1</sup> ]	0.1
$CONV_{\text{soil}}$	Conversion factor for soil concentration wet-dry weight soil	[kg <sub>wwt</sub> .kg <sub>dwt</sub> <sup>-1</sup> ]	Equation 92

$RHO_{soil}$	Bulk density of wet soil	$[kg_{wwt}.m^{-3}]$	1700
$F_{solid}$	Volume fraction of solids in soil	$[m^3.m^{-3}]$	0.6
$RHO_{solid}$	Density of solid phase	$[kg_{dwt}.m^{-3}]$	2500
$C_{soil\ porewater}$	Local concentration in soil porewater over a 180d time weighted average period	$[mg.L^{-1}]$	Equation 43
$PEC_{regional\ agric.\ soil}$	Regional predicted environmental concentration in agricultural soil	$[mg.kg_{wwt}^{-1}]$	Input (calculated outside LET) otherwise assumed to be 0
$K_{soil-water}$	Soil-water partitioning coefficient	$[mg.m^{-3}]$	Equation 37
$TWAC_{soil(180d)}$	Local concentration in soil over a 180d time weighted average period	$[mg.kg_{wwt}^{-1}]$	Equation 35
$C_{earthworm}$	Concentration in earthworm on wet weight basis	$[mg.kg_{wet\ earthworm}^{-1}]$	
$PEC_{oral,\ predator}$	Predicted environmental concentration in food	$[mg.kg_{wet\ earthworm}^{-1}]$	

For the terrestrial secondary poisoning assessment, the PEC soil is averaged over 180 days in accordance with the EU-TGD (2003) and ECHA R.16 guidance (2016). The regional PEC in agricultural soil is used to estimate the background concentration at the local scale rather than the regional PEC in natural soil. The regional PEC in agricultural soil includes contributions from aerial deposition and application of sewage sludge, which ensures a more conservative assessment of exposure of terrestrial predators to a co-formulant.

As with the secondary poisoning assessment *via* the aquatic food chain, the secondary poisoning assessment for terrestrial predators calculated in Equation 91 reflects a situation where the terrestrial predator consumes 100% of its food from the local environment. In reality, this is unlikely.

Where regional PECs in soil and porewater are available, it is assumed that 50% of a predator's diet comes from the local scale and 50% is assumed to come from the regional area (Equation 95).

In the case where a regional concentration is available, the following equation is used:

$$PEC_{oral,predator}(earthworm) = C_{earthworm} = (BCF_{earthworm} \times 0.5 \times (PEC_{porewater,sec.poisoning} + PEC_{regionalagric.soil\ porewater}) + 0.5 \times (PEC_{soil,sec.poisoning} + PEC_{regionalagric.soil}) \times F_{gut} \times CONV_{soil}) / (1 + F_{gut} \times CONV_{soil})$$

Equation 95

Where 50% of the predator's diet is assumed to come from the regional scale, the regional PEC in agricultural porewater is used to estimate the PEC in porewater at the regional scale. Where regional PECs are used to estimate the background porewater concentration at the local scale, this is estimated from the regional PEC in soil (rather than the regional PEC in porewater) in accordance with the EU-TGD (2003) and ECHA R.16 guidance (2016).

### 3.6.5 Humans exposed indirectly via the environment model

According to the ECHA REACH guidance R.16 (2016), a detailed assessment of exposure to humans via the environment is normally required if:

- Tonnage > 1000 tonnes/year or

- Tonnage > 100 tonnes/year and the substance is classified as:
  - STOT RE 1 or
  - Carcinogen or mutagen (any category) or
  - Toxic to reproduction (categories 1A or 1B)

In the case of co-formulants used in plant protection products, the CLE LET provides a screening assessment to estimate local exposure to humans from the environment. The LET will automatically calculate exposure to humans via the environment, but the results will only be used if General Population DNELs (systemic effects, long term) for inhalation and oral routes are entered by the user.

The approach that has been adopted follows the standard REACH framework closely with the same routes of exposure considered (inhalation of air and intake from drinking water, crops, meat, milk and fish). For some routes, the approach has been adapted to provide a more appropriate assessment for co-formulants which are applied to a local field, rather than at an industrial site or within a STP catchment.

The REACH R.16 (2016) guidance clearly states that for assessing exposure to humans via the environment, the local scale represents a worst-case scenario as people do not consume 100% of their diet from within the immediate vicinity of a point source. However, it is possible that people consume multiple crops treated with a co-formulant and it may be that the regional scale humans via environment assessment is not conservative enough in this situation.

The following approach has been developed to provide a simple screening assessment and is not intended to provide realistic estimates of exposure. Food consumption can vary greatly between individuals, within countries and between different member states. To avoid compounding too much conservatism, the assessment is conducted for adults, assumed to weigh 60 kg. There are more sophisticated models available to estimate exposure and if this approach identifies an area of potential concern, this should be investigated further with a more appropriate model. For example, intake via local drinking water is partly estimated from a simple porewater calculation whereas more sophisticated regulatory models for predicting groundwater exposure for PPP are available. These models should be investigated further if a risk is identified for a co-formulant using this screening approach.

The approach within the LET considers exposure to humans from the following routes:

- Inhalation via local concentration in air
- Oral intake via local drinking water
- Oral intake via treated crops
- Oral intake via milk
- Oral intake via meat
- Oral intake via fish

#### 3.6.5.1 *Inhalation via local concentration in air*

The ECHA R.16 guidance (2016) and the EU-TGD (2003b) estimate local scale inhalation exposure to humans via the environment from the annual average concentration in air at 100 metres from an industrial emission source or STP. This approach assumes release is from a point source at 10 metres height which is intended to represent release from industrial sites or wastewater treatment plants. This was not considered representative of co-formulants applied to an agricultural field where release is much closer to ground level, from an area rather than point source, dependent on the number of applications and is not continuous. Instead, the concentration in air was estimated using the approach outlined in USES version 4.0 for atmospheric emissions of pesticides (RIVM, VROM, VWS (2002)). The USES approach is based on an atmospheric plume model, PALNAT (a Dutch adapted version of the American EPA PAL model). The PALNAT model was parameterised with an area source (1 ha), emission height of 0 meters, emission strength 1 kg/m<sup>2</sup>/d and receptor point 10 metre downwind and estimates the concentration in air 10 meters downwind from an agricultural field.

$$DOSE_{\text{pest}} = AR / (A_{\text{field}} \times 1000)$$

Equation 96

## Explanation of symbols

$AR$	Application rate for co-formulant	[g.ha <sup>-1</sup> ]	User input
$A_{field}$	Area of 1 hectare field	[ha.m <sup>-2</sup> ]	10000
$DOSE_{pest}$	Single dose of pesticide	[kg.m <sup>-2</sup> ]	

The emission of a co-formulant from the treated field is estimated from its application density and the fraction of the applied dose that is emitted to air. Generalised total emission factors were defined in USES, along with the initial 24-hour averaged source strength corresponding to an application density of 1 kg per m<sup>2</sup> per application for the field use of a PPP. The initial 24-hour averaged source strength assumes that 90% of the total emission will occur during the first day after the application of a PPP, which is considered a realistic worst-case assumption. The 24-hour averaged source strengths are vapour pressure dependent and are reported in Table 29.

**Table 29:** 24-hour source strengths for field use of pesticides (RIVM, VROM, VWS (2002))

Vapour pressure at 25 °C (Pa)	24 hour averaged source strength (kg.m <sup>-2</sup> .d <sup>-1</sup> )
≥ 0.01	0.9
≥ 0.001 - 0.01	0.45
≥ 0.0001 - 0.001	0.18
≥ 0.00001 - 0.0001	0.09
< 0.00001	0.009

The source strengths reported in Table 29 represent an application density of 1 kg per m<sup>2</sup> and are converted to the expected 24-hour emission strength following application using Equation 97.

$$E_{field,air,24h} = E_{std,field,air,24h} / 1 \times DOSE_{pest} \quad \text{Equation 97}$$

## Explanation of symbols

$E_{std,field,air,24h}$	Standard 24-hour emission strength of the field	[kg.m <sup>-2</sup> .d <sup>-1</sup> ]	Table 29
1	Standard dose of source strength	[kg.m <sup>-2</sup> ]	
$DOSE_{pest}$	Single dose of pesticide	[kg.m <sup>-2</sup> ]	Equation 96
$E_{field,air,24h}$	24-hour emission strength of the field	[kg.m <sup>-2</sup> .d <sup>-1</sup> ]	

The PALNAT model estimates the concentration in air as a one-hour averaged concentration at 10 metres downwind of the field. As a worst case, if the wind direction and wind speed remain constant over 24 hours, the 24-hour averaged concentration in air is the same as the one-hour averaged concentration, as the dispersion coefficients used in the model are independent of averaging time. The 24-hour averaged concentration in air, 10 metres down wind of the field is calculated using Equation 98.

$$C_{field,air,24h} = E_{field,air,24h} / 1 \times C_{std,field,air,1h} \quad \text{Equation 98}$$

## Explanation of symbols

$E_{field,air,24 h}$	24-hour emission strength of the field	[kg.m <sup>-2</sup> .d <sup>-1</sup> ]	Equation 97
1	Standard source strength	[kg.m <sup>-2</sup> .d <sup>-1</sup> ]	
$C_{std,field,air,1 h}$	1 hour averaged concentration at 10 metres downwind of field with a standard source strength	[kg.m <sup>-3</sup> ]	1.28 x 10 <sup>-4</sup>
$C_{field,air,24 h}$	24 hour averaged concentration at 10 metres downwind of field	[kg.m <sup>-3</sup> ]	

The daily concentration in air is calculated from the 24-hour averaged concentration in air and, if available, the regional PEC in air. This is a worst-case assessment as it assumes humans are exposed within 24 hours and 10 metres downwind of the application which is extremely unlikely. The daily concentration in air is calculated using Equation 99.

$$C_{daily,air} = (C_{field,air,24h} \times 1000000) + PEC_{regional,air} \quad \text{Equation 99}$$

## Explanation of symbols

$C_{field,air,24 h}$	24-hour averaged concentration at 10 metres downwind of field	[kg.m <sup>-3</sup> ]	Equation 98
$PEC_{regional,air}$	Regional PEC in air	[mg.m <sup>-3</sup> ]	Input (calculated outside LET) otherwise assumed to be 0
$C_{daily,air}$	Daily concentration in air	[mg.m <sup>-3</sup> ]	

The LET allows a user to input the General Population, systemic effects, long term inhalation DNEL in either mg/m<sup>3</sup> or mg/kg bw/day.

If the General Population, systemic effects, long term inhalation DNEL is in mg/m<sup>3</sup>, the daily dose via inhalation is calculated using Equation 100. If the General Population, systemic effects, long term inhalation DNEL is entered in mg/kg bw/day, the daily dose via inhalation is calculated using Equation 101.

$$DOSE_{air} = C_{daily,air} \quad \text{Equation 100}$$

$$DOSE_{air} = C_{daily,air} \times F_{resp} \times IH_{air} / BW \times BIO_{inh} / BIO_{oral} \quad \text{Equation 101}$$

## Explanation of symbols

$C_{daily,air}$	Daily concentration in air	[mg.m <sup>-3</sup> ]	Equation 99
$F_{resp}$	Respirable fraction of inhaled substance	[-]	1
$IH_{air}$	Daily intake of air	[m <sup>3</sup> .d <sup>-1</sup> ]	20
$BW$	Bodyweight	[kg]	60

$BIO_{inh}$	Bioavailability by inhalation	[-]	1
$BIO_{oral}$	Bioavailability by oral route	[-]	1
$DOSE_{air}$	Daily dose via inhalation	$[mg.m^{-3}]$ $[mg.kg^{-1}.d^{-1}]$	or

### 3.6.5.2 Oral intake via local drinking water

In line with the ECHA R.16 guidance (2016) and the EU-TGD (2003b), two sources of drinking water are considered available at the local scale: groundwater and surface water. The LET predicts concentrations in local groundwater in accordance with the ECHA R.16 guidance (2016) and EU TGD (2003b) approach, by calculating the concentration in the soil pore water from the concentration in soil. The pore water concentration is then used as the worst-case concentration in groundwater below a field treated with a PPP. This approach follows a standard REACH assessment, rather than a standard agrochemical groundwater assessment which would use more sophisticated groundwater models. Consequently, this approach for estimating the groundwater concentration should not be viewed as representative and is highly conservative. If a potential risk is identified more appropriate groundwater models used for predicting PPP exposure (e.g., PEARL) should be used.

The LET also predicts the concentration in local surface water, which is represented by a ditch adjacent to an agricultural field receiving the co-formulant following exposure from spray-drift, run-off and drainage. Local surface water concentration is calculated using the agrochemical FOCUS Step 2 model discussed in Section 3.6.3. A purification factor is applied to the maximum concentration in surface water in line with the EU TGD (2003b) and EUSES 2.1. Again, this is a highly conservative assessment of the concentration in surface water used for drinking water, as it represents the maximum concentration in an edge of field water body with no dilution or averaging period considered. The highest concentration predicted in groundwater or surface water is then used for the local drinking water assessment.

As the drinking water concentrations calculated in the LET are based on a single treated agricultural field with a surface area of 1 ha, the predicted concentration in local groundwater and surface water is likely to over-predict the local exposure to humans via the environment and is not considered representative of drinking water sources. An approach similar to that applied in the secondary poisoning assessment has, therefore, been adopted where:

- 50% of consumed drinking water comes from local sources (for which the maximum local concentration in groundwater or surface water is selected)
- 50% of consumed drinking water comes from regional sources (for which maximum regional concentration in groundwater or surface water is selected)

The local concentration in soil at 180 days is used to estimate the PEC in groundwater using Equation 102.

$$PEC_{local_{gw\_dw}} = TWAC_{soil(180d)} \times RHO_{soil} / (K_{soil-water} \times 1000) + PEC_{regional_{porewater}} \quad \text{Equation 102}$$

#### Explanation of symbols

$TWAC_{soil(180d)}$	Local concentration in soil (wet weight) as a 180d time weighted average	$[mg.kg_{wwt}^{-1}]$	Equation 36
$RHO_{soil}$	Bulk density of wet soil	$[kg.m^{-3}]$	1700
$K_{soil-water}$	Soil-water partitioning coefficient	$[m^3.m^{-3}]$	Equation 37
$PEC_{regional_{porewater}}$	Regional PEC in porewater	$[mg.L^{-1}]$	Input (calculated outside LET)

otherwise  
assumed to be 0

$PEC_{local, gw\_dw}$  Predicted environmental concentration in soil porewater (drinking water) [mg.L<sup>-1</sup>]

The local concentration in drinking water is estimated using Equation **103** and the purification factor is calculated using Equation **104**.

$$PEC_{local, sw\_dw} = (C_{local, sw\_max}) / 1000 \times F_{pur} \quad \text{Equation 103}$$

Explanation of symbols

$C_{local, sw\_max}$	Maximum local freshwater concentration	[µg.L <sup>-1</sup> ]	Equation 69
$F_{pur}$	Purification factor for surface water	[-]	Equation 104
$PEC_{local, sw\_dw}$	Predicted environmental concentration in surface water (drinking water)	[mg.L <sup>-1</sup> ]	

$$F_{pur} = \max(F_{sys1, pur}, F_{sys2, pur}) \quad \text{Equation 104}$$

Explanation of symbols

$F_{sys1, pur}$	Purification factor system 1	[-]	Table 30
$F_{sys2, pur}$	Purification factor system 2	[-]	Table 30
$F_{pur}$	Purification factor for surface water	[-]	

Table 30: Purification factors (EU-TGD, 2003b)

Treatment process	Log Kow			Henry's Law constant (Pa.m <sup>3</sup> .mol <sup>-1</sup> )		Aerobic biodegradation rate (days)	
	<4	4-5	>5	≤100	>100	>10	≤10
System 1 (open reservoirs)	1	¼	1/16	1	½	1	1
System 2 (dune recharge)	1	½	¼	1	½	1	¼

The local concentration in drinking water represents the highest concentration predicted in local groundwater or surface water and is calculated using Equation **105**.

$$CONC_{drw, L} = \max(PEC_{local, gw\_dw}, PEC_{local, sw\_dw}) \quad \text{Equation 105}$$

Explanation of symbols

$PEC_{local, gw\_dw}$	Predicted environmental concentration in soil porewater (drinking water)	[mg.L <sup>-1</sup> ]	Equation 102
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$PEC_{local,sw,dw}$	Predicted environmental concentration in surface water (drinking water)	[mg.L <sup>-1</sup> ]	Equation 103
$CONC_{drw,L}$	Local concentration in drinking water	[mg.L <sup>-1</sup> ]	

If regional PECs are not available, then the daily dose via drinking water is calculated using Equation **106**.

$$DOSE_{drw} = CONC_{drw,L} \times IH_{drw} / BW \quad \text{Equation 106}$$

Explanation of symbols

$CONC_{drw,L}$	Local concentration in drinking water	[mg.L <sup>-1</sup> ]	Equation 105
$IH_{drw}$	Daily intake of drinking water	[L.d <sup>-1</sup> ]	2
$BW$	Bodyweight	[kg]	60
$DOSE_{drw}$	Daily dose via drinking water	[mg.kg <sup>-1</sup> .d <sup>-1</sup> ]	

If regional PECs are available, the regional concentration in drinking water is calculated using the same approach as for local scale drinking water, using Equation **107**.

$$CONC_{drw,R} = \max(PEC_{regional,soil\ porewater}, (PEC_{regional,sw} \times F_{pur})) \quad \text{Equation 107}$$

Explanation of symbols

$PEC_{regional,soil\ porewater}$	Regional predicted environmental concentration in agricultural soil porewater	[mg.L <sup>-1</sup> ]	Input (calculated outside LET) otherwise assumed to be 0
$PEC_{regional,sw}$	Regional predicted environmental concentration in surface water	[mg.L <sup>-1</sup> ]	Input (calculated outside LET) otherwise assumed to be 0
$F_{pur}$	Purification factor for surface water	[-]	Equation 104
$CONC_{drw,R}$	Regional concentration in drinking water	[mg.L <sup>-1</sup> ]	

The daily dose via drinking water is then calculated assuming 50% of drinking water comes from local scale sources and 50% of drinking water comes from regional scale sources:

$$DOSE_{drw} = (0.5 \times CONC_{drw,L} + 0.5 \times CONC_{drw,R}) \times IH_{drw} / BW \quad \text{Equation 108}$$

Explanation of symbols

$CONC_{drw,L}$	Local concentration in drinking water	[mg.L <sup>-1</sup> ]	Equation 105
$CONC_{drw,R}$	Regional concentration in drinking water	[mg.L <sup>-1</sup> ]	Equation 107
$IH_{drw}$	Daily intake of drinking water	[L.d <sup>-1</sup> ]	2
$BW$	Bodyweight	[kg]	60

$DOSE_{drv}$	Daily dose via drinking water	[mg.kg <sup>-1</sup> .d <sup>-1</sup> ]
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### 3.6.5.3 Oral intake via crops

ECHA R.16 (2016) and the EU-TGD (2003b) estimate local scale exposure to humans from crops following indirect exposure. Exposure is assumed to be by chemical uptake by plant roots or leaves and is considered a passive process. The model is a simplistic estimation of plant uptake and only estimates exposure in the leaf and root tissue and does not account for concentrations in the fruit.

Exposure from co-formulants to the crop could be via these indirect processes, where application is directly to the soil. However, it is also possible that the crop is directly exposed during application. Many factors can influence the potential residue concentration in crops, including substance properties, type of application (e.g., spray, granules), application timing (e.g., BBCH), PPP function (e.g., insecticide, herbicide), crop type, harvest timing and environmental conditions.

Considering the differences between the standard REACH assessment and potential pathways for co-formulants, an alternative approach has been developed to estimate potential exposure to humans via treated crops. This approach has been integrated in the LET and was developed to be a conservative screening approach, using standard data required for REACH registrations (i.e., physical chemical parameters and general population DNELs). It has been assumed that the GAP and specific information such as foliar half-lives of co-formulants are not available and, therefore, the following assessment is not intended to reflect expected levels of co-formulant in crops when consumed. However, it does provide a screening assessment which, if a potential concern is identified, would provide a starting point to consider additional factors that influence co-formulant exposure to crops.

For the screening assessment, only non-volatile co-formulants are expected to contribute to exposure in the crop. Substances with a vapour pressure of  $\geq 0.01$  Pa applied as sprays are expected to evaporate from the treated crops within 24 hours of application and the potential to be transferred into the treated crop is very limited.

For non-volatile co-formulants, a simplified approach is adopted following a general method for predicting residues in treated crops described by Maclachlan and Hamilton (2010). This method is applicable for formulations applied as sprays, granules or treated seeds. The total amount of an applied co-formulant (in kg/ha) is related to the total yield of a crop obtained from the treated 1-hectare field (in t/ha), and a potential maximum residual concentration in the crop is thus calculated. Maclachlan and Hamilton (2010) consider a factor,  $f_{commodity}$ , which describes the fraction of the applied PPP that is likely to reach the treated commodity and thus the harvested crop. This approach doesn't consider additional factors that may affect residue concentrations such as substance breakdown between application and harvest or post-harvest processing (e.g., washing or peeling fruit/vegetables).

The EU TGD approach considers only two types of treated crops, leafy and root vegetables, when predicting indirect exposure of man via the environment. The approach included in the LET, considers a wider range of treated crops, including pome and stone fruits, citrus, berries, table grapes, cereals, pulses, oil seeds, root vegetables, leafy vegetables, bulb vegetables, brassica vegetables and tomatoes.

Following the approach described by Maclachlan and Hamilton (2010), crop yield, crop intake and  $f_{commodity}$  were defined for each of these crops.

The crop yield for the individual crops was determined from EUROSTAT and represents the average yield for the individual crops across 28 EU member states from 2011 to 2019. The approach is explained in more detail in Appendix 2: and the crop yields are reported in Table 32.

Human consumption of the individual crops was estimated using the maximum food intake across adult diets in 16 member states and 6 GEMS/Food Cluster diets relevant for the EU Member States used in the EFSA PRIMo v3 model for chronic exposure assessments alongside the corresponding average body weight for the relevant dataset (see Appendix 3:). The daily crop consumption values reported in Table 32 should be considered conservative. They represent the maximum average consumption for crops that were selected to represent the highest average food consumption for that crop category.

Maclachlan and Hamilton (2010) define  $f_{\text{commodity}}$  as the fraction of application that is intercepted by the commodity of interest and calculated  $f_{\text{commodity}}$  as commodity surface area/crop leaf surface area. Where  $f_{\text{commodity}}$  values were reported by Maclachlan and Hamilton (2010), these were used in the LET. Where no data was available, the authors assumed a default  $f_{\text{commodity}}$  of 1.0 for crops where the entire above ground plant is the commodity and 0.1 for crops where the fruit is the commodity. This approach was also adopted in the LET for crops where  $f_{\text{commodity}}$  was not reported by Maclachlan and Hamilton (2010). The basis for the  $f_{\text{commodity}}$  values used in the LET are summarised in Table 31.

**Table 31:**  $f_{\text{commodity}}$  values selected for treated crops in CLE LET

Crop	$f_{\text{commodity}}$	
Pome/stone fruit	0.079	Maclachlan and Hamilton (2010), Apple
Citrus	0.0819	Maclachlan and Hamilton (2010), Lemons/mandarin
Berries	0.16	Maclachlan and Hamilton (2010), Table/wine grapes
Table grapes	0.16	Maclachlan and Hamilton (2010), Table grapes
Cereals	0.1	Extrapolated from Maclachlan and Hamilton (2010)
Pulses	0.21	Maclachlan and Hamilton (2010), Peas plus pod
Oil seeds (rapeseed)	0.1	Extrapolated from Maclachlan and Hamilton (2010)
Root vegetables	0.1	Extrapolated from Maclachlan and Hamilton (2010)
Leafy vegetables	1	Maclachlan and Hamilton (2010), Lettuce/spinach
Bulb vegetables	1	Maclachlan and Hamilton (2010), Leeks/shallots
Tomatoes	0.082	Maclachlan and Hamilton (2010), Field tomato
Brassica vegetables	0.1	Extrapolated from Maclachlan and Hamilton (2010)

A summary of the crop yield, daily crop intake and  $f_{\text{commodity}}$  values used in the calculation of oral intake of a non-volatile co-formulant via treated crops, are reported in Table 32.

**Table 32:** Parameters used in the calculation of oral exposure to co-formulants via consumption of treated crops

Crop	Crop yield (t/ha)	Daily crop consumption (kg/day)	$f_{\text{commodity}}$
Pome/stone fruit	20.1	0.1968	0.079
Citrus	21.4	0.1461	0.0819
Berries	4.3	0.0135	0.16
Table grapes	9.8	0.0631	0.16
Cereals	5.4	0.4341	0.1
Pulses	5.3	0.0238	0.21
Oil seeds (rapeseed)	2.9	0.0327	0.1
Root vegetables	41.6	0.3200	0.1
Leafy vegetables	23.0	0.0371	1
Bulb vegetables	30.9	0.0454	1
Tomatoes	68.0	0.2148	0.082

Crop	Crop yield (t/ha)	Daily crop consumption (kg/day)	f <sub>commodity</sub>
Brassica vegetables	28.9	0.0126	0.1

The concentration in the harvested crop is a function of application rate, crop yield and the fraction of the crop that is the commodity. It is calculated using Equation 109.

$$CONC_{crop,i} = AR \times N_{app} / CROP_{yield,i} \times f_{commodity,i} \quad \text{Equation 109}$$

$i \in \{\text{pome/stone fruit, citrus, berries, table grapes, cereals, pulses, oilseeds, root vegetables, leafy vegetables, bulb vegetables, tomatoes, brassica vegetables}\}$

Explanation of symbols

<i>AR</i>	Application rate for co-formulant	[g.ha <sup>-1</sup> ]	User input
<i>N<sub>app</sub></i>	Number of application events	[-]	User input
<i>CROP<sub>yield,i</sub></i>	Crop yield	[t.ha <sup>-1</sup> ]	Table 32
<i>f<sub>commodity,i</sub></i>	Commodity fraction of crop	[-]	Table 32
<i>CONC<sub>crop,i</sub></i>	Concentration in harvested crop	[mg.kg <sup>-1</sup> ]	

Daily intake of each treated crop is calculated using Equation 110.

$$INTAKE_{crop,i} = CROP_{intake,i} \times CONC_{crop,i} / BW \quad \text{Equation 110}$$

$i \in \{\text{pome/stone fruit, citrus, berries, table grapes, cereals, pulses, oilseeds, root vegetables, leafy vegetables, bulb vegetables, tomatoes, brassica vegetables}\}$

Explanation of symbols

<i>CROP<sub>intake,i</sub></i>	Daily crop consumption	[kg.day <sup>-1</sup> ]	Table 32
<i>CONC<sub>crop,i</sub></i>	Concentration in harvested crop	[mg.kg <sup>-1</sup> ]	Equation 109
<i>BW</i>	Bodyweight	[kg]	60
<i>INTAKE<sub>crop,i</sub></i>	Daily intake per crop	[mg.kg <sup>-1</sup> .day <sup>-1</sup> ]	

If application is a spray and vapour pressure at 25 °C is  $\geq 0.01$  Pa:

$$DOSE_{crop} = 0 \quad \text{Equation 111}$$

Explanation of symbols

<i>DOSE<sub>crop</sub></i>	Daily dose via crops	[mg.kg <sup>-1</sup> .d <sup>-1</sup> ]
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For all other application types and for sprays where vapour pressure at 25 °C is  $< 0.01$  Pa:

$$DOSE_{crop} = \sum INTAKE_{crop,i} \quad \text{Equation 112}$$

$i \in \{\text{pome/stone fruit, citrus, berries, table grapes, cereals, pulses, oilseeds, root vegetables, leafy vegetables, bulb vegetables, tomatoes, brassica vegetables}\}$

#### Explanation of symbols

$INTAKE_{crop,i}$	Daily intake from crops of $i$	$[\text{mg.kg}^{-1}.\text{day}^{-1}]$	Equation 110
$DOSE_{crop}$	Daily dose via treated crops	$[\text{mg.kg}^{-1}.\text{d}^{-1}]$	

#### 3.6.5.4 Oral intake via milk and meat

ECHA R.16 guidance (2016) and the EU-TGD (2003b) outline an approach for estimating local scale exposure to humans from consumption of meat and dairy products. It assumes that cattle are exposed to chemicals in grass and soil, drinking water and inhalation of air. The same approach has been adopted in the LET, but adjusted to assume cattle eat treated crops as fodder, rather than grass.

##### 3.6.5.4.1 Intake through fodder

The concentration in fodder is calculated by dividing the maximum application rate (kg/ha) that reaches the treated crop by the harvested yield of forage crops (t/ha) derived from EUROSTAT (Appendix 2:). To ensure a worst-case assessment it is assumed the fodder crop intercepts 100% of the application and cattle consume all of the crop (i.e.,  $f_{commodity}$  is 1).

$$C_{crop,fodder} = AR \times N_{app} \times f_{int} \times f_{commodity\ fodder} / Y_{commodity} \quad \text{Equation 113}$$

#### Explanation of symbols

$AR$	Application rate for co-formulant	$[\text{g.ha}^{-1}]$	User input
$N_{app}$	Number of application events	$[-]$	User input
$f_{int}$	Fraction intercepted by feeding crops	$[-]$	1
$f_{commodity\ fodder}$	Commodity fraction of fodder crops	$[-]$	1
$Y_{commodity}$	Yield of feeding crops	$[\text{t.ha}^{-1}]$	14.7
$C_{crop,fodder}$	Concentration in fodder crops	$[\text{mg.kg}_{wwt}^{-1}]$	

It has been assumed that the daily intake of grass by cattle is equivalent to the daily intake of fodder crops, and the daily intake of grass by cattle is calculated using Equation 114.

$$IC_{grass} = IC_{dwt,grass} \times CONV_{grass} \quad \text{Equation 114}$$

#### Explanation of symbols

$IC_{dwt,grass}$	Daily intake of grass (dry weight)	$[\text{kg}_{dwt}.\text{day}^{-1}]$	16.9
$CONV_{grass}$	Conversion dry to wet weight grass	$[\text{kg}_{wwt}.\text{kg}_{dwt}^{-1}]$	4
$IC_{grass}$	Daily intake of grass (wet weight)	$[\text{kg}_{wwt}.\text{day}^{-1}]$	

##### 3.6.5.4.2 Intake through soil

In keeping with the ECHA R.16 guidance (2016) and the EU-TGD (2003b), intake of soil by cattle during grazing has been included in the assessment. However, this is a conservative assessment as cattle

consuming fodder are likely to be indoors and not grazing outdoors. The local concentration in soil is taken as the 180-day time weighted average (Equation 115).

$$C_{\text{soil}} = C_{\text{local,soil,humans via env}} + PEC_{\text{regional agr.soil}} \quad \text{Equation 115}$$

#### Explanation of symbols

$C_{\text{local,soil,humans via env}}$	Local concentration in soil (wet weight) used in humans via the environment calculations (180d time weighted average)	[mg.kg <sub>wwt</sub> <sup>-1</sup> ]	Equation 36
$PEC_{\text{regional agr.soil}}$	Regional concentration in agricultural soil	[mg.kg <sub>wwt</sub> <sup>-1</sup> ]	Input (calculated outside LET) otherwise assumed to be 0
$C_{\text{soil}}$	Concentration in soil	[mg.kg <sub>wwt</sub> <sup>-1</sup> ]	

The daily intake of soil by cattle is calculated using Equation 116.

$$IC_{\text{soil}} = IC_{\text{dwt,soil}} \times CONV_{\text{soil}} \quad \text{Equation 116}$$

#### Explanation of symbols

$IC_{\text{dwt,soil}}$	Daily intake of soil (dry weight)	[kg <sub>dwt</sub> .day <sup>-1</sup> ]	0.41
$CONV_{\text{soil}}$	Conversion factor for soil concentration wet-dry weight soil	[kg <sub>wwt</sub> .kg <sub>dwt</sub> <sup>-1</sup> ]	Equation 92
$IC_{\text{soil}}$	Daily intake of soil (wet weight)	[kg <sub>wwt</sub> .day <sup>-1</sup> ]	

#### 3.6.5.4.3 Intake through air

As a worst case, it has been assumed that cattle inhale air within 24 hours and 10 meters downwind of a treated field. In reality, cattle would not be exposed to this level of co-formulant exposure on a daily basis.

$$C_{\text{air}} = C_{\text{daily,air}} \quad \text{Equation 117}$$

#### Explanation of symbols

$C_{\text{daily,air}}$	Daily concentration in air	[mg.m <sup>-3</sup> ]	Equation 99
$C_{\text{air}}$	Concentration in air	[mg.m <sup>-3</sup> ]	

#### 3.6.5.4.4 Intake through drinking water

It is assumed that cattle drink water from the same local sources as humans exposed via the environment using Equation 118. However, to account for a situation where cattle could drink directly from a waterbody, the contribution from regional sources has not been included in the assessment for cattle.

$$C_{\text{drw}} = \max(PEC_{\text{local,gw,dw}}, PEC_{\text{local,sw,dw}}) \quad \text{Equation 118}$$

## Explanation of symbols

$PEC_{local, gw\_dw}$	Predicted environmental concentration in soil porewater (drinking water)	[mg.L <sup>-1</sup> ]	Equation 102
$PEC_{local, sw\_dw}$	Predicted environmental concentration in surface water (drinking water)	[mg.L <sup>-1</sup> ]	Equation 103
$C_{drw}$	Concentration in drinking water	[mg.L <sup>-1</sup> ]	

## 3.6.5.4.5 Dose in dairy products

The concentration in milk is calculated by applying a biotransfer factor to the diet of the cattle covering intake from air, soil, fodder crops and drinking water. The biotransfer or bioaccumulation factor for milk is calculated from log Kow according to Table 33.

**Table 33:** Bioaccumulation factor for milk (EU TGD (2003b), EUSES 2.1)

	Log Kow		
	< 3	≥ 3 - ≤ 6.5	> 6.5
BAF <sub>milk</sub>	10 <sup>-8.1+3</sup>	10 <sup>-8.1+log Kow</sup>	10 <sup>-8.1+6.5</sup>

$$C_{milk} = BAF_{milk} \times (IC_{grass} \times C_{crop, fodder} + IC_{soil} \times C_{soil} + IC_{air} \times C_{air} + IC_{drw} \times C_{drw}) \quad \text{Equation 119}$$

## Explanation of symbols

$BAF_{milk}$	Bioaccumulation factor for milk	[day.kg <sub>milk</sub> <sup>-1</sup> ]	Table 33
$IC_{grass}$	Daily intake of grass (wet weight)	[kg <sub>wwt</sub> .day <sup>-1</sup> ]	Equation 114
$C_{crop, fodder}$	Concentration in fodder crops	[mg.kg <sub>wwt</sub> <sup>-1</sup> ]	Equation 113
$IC_{soil}$	Daily intake of soil (wet weight)	[kg <sub>wwt</sub> .day <sup>-1</sup> ]	Equation 116
$C_{soil}$	Concentration in soil	[mg.kg <sub>wwt</sub> <sup>-1</sup> ]	Equation 115
$IC_{air}$	Daily inhalation rate of cattle	[m <sup>3</sup> .day <sup>-1</sup> ]	122
$C_{air}$	Concentration in air	[mg.m <sup>-3</sup> ]	Equation 117
$IC_{drw}$	Daily intake of drinking water for cattle	[L.day <sup>-1</sup> ]	55
$C_{drw}$	Concentration in drinking water	[mg.L <sup>-1</sup> ]	Equation 118
$C_{milk}$	Concentration in milk	[mg.kg <sub>milk</sub> <sup>-1</sup> ]	

The daily dose through intake of dairy products is then calculated using Equation 120.

$$DOSE_{dairy} = C_{milk} \times IH_{milk} / BW \quad \text{Equation 120}$$

## Explanation of symbols

$C_{milk}$	Concentration in milk	[mg.kg <sub>milk</sub> <sup>-1</sup> ]	Equation 119
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$IH_{milk}$	Daily intake of dairy products	[kg <sub>milk</sub> .d <sup>-1</sup> ]	0.561
$BW$	Bodyweight	[kg]	60
$DOSE_{dairy}$	Daily dose via dairy products	[mg.kg <sup>-1</sup> .d <sup>-1</sup> ]	

### 3.6.5.4.6 Dose in meat products

The concentration in meat products is also calculated by applying a biotransfer factor to the diet of the cattle covering intake from air, soil, fodder crops and drinking water. The biotransfer or bioaccumulation factor for meat is calculated from log Kow according to Table 32).

**Table 34:** Bioaccumulation factor for meat (EU TGD (2003b), EUSES 2.1)

	Log Kow		
	< 1.5	≥ 1.5 - ≤ 6.5	> 6.5
$BAF_{meat}$	$10^{-7.6+1.5}$	$10^{-7.6+\log Kow}$	$10^{-7.6+6.5}$

$$C_{meat} = BAF_{meat} \times (IC_{grass} \times C_{crop,fodder} + IC_{soil} \times C_{soil} + IC_{air} \times C_{air} + IC_{drw} \times C_{drw}) \quad \text{Equation 121}$$

#### Explanation of symbols

$BAF_{meat}$	Bioaccumulation factor for meat	[day.kg <sub>meat</sub> <sup>-1</sup> ]	Table 34
$IC_{grass}$	Daily intake of grass (wet weight)	[kg <sub>wwt</sub> .day <sup>-1</sup> ]	Equation 114
$C_{crop,fodder}$	Concentration in fodder crops	[mg.kg <sub>wwt</sub> <sup>-1</sup> ]	Equation 113
$IC_{soil}$	Daily intake of soil (wet weight)	[kg <sub>wwt</sub> .day <sup>-1</sup> ]	Equation 116
$C_{soil}$	Concentration in soil	[mg.kg <sub>wwt</sub> <sup>-1</sup> ]	Equation 115
$IC_{air}$	Daily inhalation rate of cattle	[m <sup>3</sup> .day <sup>-1</sup> ]	122
$C_{air}$	Concentration in air	[mg.m <sup>-3</sup> ]	Equation 117
$IC_{drw}$	Daily intake of drinking water for cattle	[L.day <sup>-1</sup> ]	55
$C_{drw}$	Concentration in drinking water	[mg.L <sup>-1</sup> ]	Equation 118
$C_{meat}$	Concentration in meat	[mg.kg <sub>meat</sub> <sup>-1</sup> ]	

The daily dose through intake of meat products is then calculated using Equation 122.

$$DOSE_{meat} = C_{meat} \times IH_{meat} / BW \quad \text{Equation 122}$$

#### Explanation of symbols

$C_{meat}$	Concentration in meat	[mg.kg <sub>meat</sub> <sup>-1</sup> ]	Equation 121
$IH_{meat}$	Daily intake of meat	[kg <sub>meat</sub> .d <sup>-1</sup> ]	0.301
$BW$	Bodyweight	[kg]	60
$DOSE_{meat}$	Daily dose via meat	[mg.kg <sup>-1</sup> .d <sup>-1</sup> ]	



### 3.6.5.5 Oral intake via fish

ECHA R.16 (2016) and the EU-TGD (2003b) estimate local scale exposure to humans from consuming fish as a function of the surface water concentration and a bioconcentration factor in fish. The same approach has been adopted in the LET, although instead of the annual average in surface water, a 21-day time weighted average has been used. It is, though, considered unlikely that fishing takes place in a narrow ditch which is adjacent to an agricultural field with very limited exchange of water. No dilution factor is included for the screening assessment, and this should be considered very conservative.

The bioconcentration factor (BCF) for fish can be inputted as a measured value. If this is not available, it can be estimated from log K<sub>ow</sub> using the approach discussed for secondary poisoning (Section 3.6.4). The units are converted for the humans via environment assessment using Equation 123.

$$BCF_{fish} = BCF_{fish} / 1000 \quad \text{Equation 123}$$

#### Explanation of symbols

$BCF_{fish}$	Bioconcentration factor for fish	[L.kg <sub>wet fish</sub> <sup>-1</sup> ]	Measured or estimated from log K <sub>ow</sub> (Equation 80 and Equation 81)
$BCF_{fish}$	Bioconcentration factor for fish	[m <sup>3</sup> .kg <sub>wwt</sub> <sup>-1</sup> ]	

$$C_{water} = (C_{local,sw,HvE,fish} + PEC_{regional,sw}) / 1000000 \quad \text{Equation 124}$$

#### Explanation of symbols

$C_{local,sw,HvE,fish}$	21-day time weighted average in surface water	[µg.L <sup>-1</sup> ]	Equation 78
$PEC_{regional,sw}$	Regional predicted environmental concentration in surface water	[µg.L <sup>-1</sup> ]	Input (calculated outside LET) otherwise assumed to be 0
$C_{water}$	Concentration in surface water	[kg.m <sup>3</sup> ]	

The concentration in fish consumed by humans is estimated according to Equation 125.

$$C_{fish} = BCF_{fish} \times C_{water} \times 1000000 \quad \text{Equation 125}$$

#### Explanation of symbols

$BCF_{fish}$	Bioconcentration factor for fish	[m <sup>3</sup> .kg <sub>wwt</sub> <sup>-1</sup> ]	Equation 123
$C_{water}$	Concentration in surface water	[kg.m <sup>-3</sup> ]	Equation 124
$C_{fish}$	Concentration in wet fish	[mg.kg <sub>wwt</sub> <sup>-1</sup> ]	

The daily dose through intake of fish is calculated using Equation 126.

$$DOSE_{fish} = C_{fish} \times IH_{fish} / BW \quad \text{Equation 126}$$

Explanation of symbols

$C_{fish}$	Concentration in fish	[mg.kg <sub>wwt</sub> <sup>-1</sup> ]	Equation 125
$IH_{fish}$	Daily intake of fish	[kg <sub>wwt</sub> .d <sup>-1</sup> ]	0.115
$BW$	Bodyweight	[kg]	60
$DOSE_{fish}$	Daily dose via fish	[mg.kg <sup>-1</sup> .d <sup>-1</sup> ]	

### 3.6.6 PEC and RCR Calculations

#### 3.6.6.1 PEC calculations

The calculations discussed in Section 3.6.2 to Section 3.6.3.2 are used to calculate the local concentrations of a co-formulant in soil, surface water and sediment. This accounts for exposure at the local environment following use of a co-formulant in plant protection products. However, use of co-formulants in PPP and in other sectors in the wider, regional environment should also be assessed by a regional scale assessment. This can be conducted using multi-media fate models (e.g., SimpleBox). CLE SpERCs (See Section 3.7) have been developed to allow a regional scale assessment to be conducted in models such as EUSES, CHESAR and ECETOC TRA. The regional concentrations calculated with these models can then be entered into the LET manually (e.g., EUSES, CHESAR) or imported directly into the tool (from the ECETOC TRA; see Section 3.2).

This allows the local PEC to be calculated as the sum of local concentration and regional (background) concentration. Where regional concentrations are inputted to the LET the PECs are calculated as shown in Equation 127 to Equation 131. Where regional concentrations are not available, the  $PEC_{compartment} = C_{local,compartment}$ .

#### PEC Fresh Water (Pelagic)

$$PEC_{sw} = C_{local,sw \max} + PEC_{regional,sw} \quad \text{Equation 127}$$

Explanation of symbols

$PEC_{regional,sw}$	Freshwater concentration at the regional scale	[µg.L <sup>-1</sup> ]	Calculated outside the LET
$C_{local,sw \max}$	Maximum local freshwater concentration	[µg.L <sup>-1</sup> ]	Equation 69
$PEC_{sw}$	Predicted environmental concentrations in freshwater	[µg.L <sup>-1</sup> ]	

#### PEC Fresh Water (Sediment)

$$PEC_{sed} = C_{local,sed \max} + PEC_{regional,sed} \quad \text{Equation 128}$$

Explanation of symbols

$PEC_{regional,sed}$	Freshwater sediment concentration at the regional scale (dry weight)	[µg.kg <sub>dwt</sub> <sup>-1</sup> ]	Calculated outside the LET
$C_{local,sed \max}$	Maximum local freshwater sediment concentration (dry weight)	[µg.kg <sub>dwt</sub> <sup>-1</sup> ]	Equation 70

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<i>PEC<sub>sed</sub></i>	Predicted environmental concentrations in freshwater sediment (dry weight)	[ $\mu\text{g.kg}_{\text{dwt}}^{-1}$ ]
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*PEC Marine Water (Pelagic)*

$$PEC_{\text{marine water}} = C_{\text{local}}_{\text{marine water}} + PEC_{\text{regional}}_{\text{marine water}} \quad \text{Equation 129}$$

## Explanation of symbols

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<i>PEC<sub>regional</sub></i> <sub>marine water</sub>	Marine water concentration at the regional scale	[ $\mu\text{g.L}^{-1}$ ]	Calculated outside the LET
<i>C<sub>local</sub></i> <sub>marine water</sub>	Local marine water concentration	[ $\mu\text{g.L}^{-1}$ ]	Equation 71
<i>PEC<sub>marine water</sub></i>	Predicted environmental concentration in marine water	[ $\mu\text{g.L}^{-1}$ ]	

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*PEC Marine Water (Sediment)*

$$PEC_{\text{marine sediment}} = C_{\text{local}}_{\text{marine sediment}} + PEC_{\text{regional}}_{\text{marine sediment}} \quad \text{Equation 130}$$

## Explanation of symbols

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<i>PEC<sub>regional</sub></i> <sub>marine sediment</sub>	Marine sediment concentration at the regional scale (dry weight)	[ $\mu\text{g.kg}_{\text{dwt}}^{-1}$ ]	Calculated outside the LET
<i>C<sub>local</sub></i> <sub>marine sediment</sub>	Local marine sediment concentration (dry weight)	[ $\mu\text{g.kg}_{\text{dwt}}^{-1}$ ]	Equation 72
<i>PEC<sub>marine sediment</sub></i>	Predicted environmental concentration in marine sediment (dry weight)	[ $\mu\text{g.kg}_{\text{dwt}}^{-1}$ ]	

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*PEC Soil*

$$PEC_{\text{soil}} = C_{\text{local}}_{\text{soil}} + PEC_{\text{regional}}_{\text{agric.soil}} \quad \text{Equation 131}$$

## Explanation of symbols

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<i>PEC<sub>regional</sub></i> <sub>agric.soil</sub>	Agricultural soil concentration at the regional scale (dry weight)	[ $\mu\text{g.kg}_{\text{dwt}}^{-1}$ ]	Calculated outside the LET
<i>C<sub>local</sub></i> <sub>soil</sub>	Local soil concentration (30-day TWA) (dry weight)	[ $\mu\text{g.kg}_{\text{dwt}}^{-1}$ ]	Equation 34
<i>PEC<sub>soil</sub></i>	Predicted environmental concentration in soil (dry weight)	[ $\mu\text{g.kg}_{\text{dwt}}^{-1}$ ]	

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**3.6.6.2 RCR calculations**

The risk characterisation ratios (RCRs) for each relevant environmental compartment are calculated using Equation 132.

$$RCR_{\text{compartment}} = PEC_{\text{compartment}} / PNEC_{\text{compartment}} \quad \text{Equation 132}$$

## Explanation of symbols

$PEC_{compartment}$	Predicted environmental concentrations in environmental compartment		Section 3.6.6.1
$PNEC_{compartment}$	Predicted no environmental concentrations in environmental compartment		User input
$RCR_{compartment}$	Risk Characterisation Ratio in environmental compartment	[-]	

Where the equilibrium partitioning method has been used to calculate the PNEC sediment, PNEC marine water sediment and/or PNEC soil and the log Kow is greater than 5, an additional assessment factor of 10 is applied to the corresponding RCR using Equation 133.

If  $PNEC_{compartment}$  = Equilibrium partitioning method and  $\log Kow > 5$ :

$$RCR_{compartment} = PEC_{compartment} / PNEC_{compartment} \times 10 \quad \text{Equation 133}$$

Explanation of symbols

$PEC_{compartment}$	Predicted environmental concentrations in environmental compartment		Section 3.6.6.1
$PNEC_{compartment}$	Predicted no environmental concentrations in environmental compartment		User input
$RCR_{compartment}$	Risk Characterisation Ratio in environmental compartment	[-]	

For humans via the environment, the RCR for intake by inhalation is calculated using Equation 134.

$$RCR_{inhalation} = DOSE_{air} / DNEL_{inhalation} \quad \text{Equation 134}$$

Explanation of symbols

$DOSE_{air}$	Daily dose via inhalation	$[mg \cdot m^{-3}]$ $[mg \cdot kg^{-1} \cdot d^{-1}]$	Equation 100/ Equation 101
$DNEL_{inhalation}$	General population, systemic effects, long term inhalation DNEL	$[mg \cdot m^{-3}]$ $[mg \cdot kg^{-1} \cdot d^{-1}]$	User input
$RCR_{inhalation}$	RCR inhalation	[-]	

For humans via the environment, the RCR for oral intake is calculated for each route of exposure using Equation 135.

$$RCR_{oral,i} = DOSE_i / DNEL_{oral} \quad \text{Equation 135}$$

$i \in \{\text{drinking water, crops, milk, meat, fish}\}$

Explanation of symbols

$DOSE_{oral,i}$	Daily dose via oral route i	$[mg \cdot kg^{-1} \cdot d^{-1}]$	Equation 106 or Equation 108, Equation 111 or
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			Equation 112, Equation 120, Equation 122, Equation 126
$DNEL_{oral}$	General population, systemic effects, long term oral DNEL	[mg.kg <sup>-1</sup> .d <sup>-1</sup> ]	User input
$RCR_i$	RCR oral via route i	[-]	

The overall RCR for humans via the environment is calculated using Equation 136.

$$RCR_{total} = \sum RCR_{oral,i} + RCR_{inhalation} \quad \text{Equation 136}$$

$i \in \{\text{drinking water, crops, milk, meat, fish}\}$

Explanation of symbols

$RCR_{oral,i}$	RCR oral via route i	[-]	Equation 135
$RCR_{inhalation}$	RCR inhalation	[-]	Equation 134
$RCR_{total}$	Overall RCR for humans via environment	[-]	

### 3.6.7 Estimation of the safe dose

When the LET is run in ‘Default’ assessment mode, the application rate is initially set as 1 kg.ha<sup>-1</sup>. The result of this run is not reported back but used internally by the model for an iterative calculation of the output variable ‘maximum safe dose’ (i.e., the maximum dose at which for none of the environmental compartments RCR will reach or exceed 1.0). After completion of the iteration, PECs and RCRs are reported at this application rate, and the most sensitive environmental compartment is identified. If so desired, after the initial assessment, the user can specify a customised target RCR, and exposure and application rate are recalculated at the specified RCR.

The safe dose is calculated using Equation 137 (initially AR = 1 kg.ha<sup>-1</sup>) for surface water, freshwater sediment, marine water, marine water sediment and soil. The maximum dose acceptable for the most sensitive environmental compartment for the substance assessed is reported as the estimated safe dose.

$$\text{SafeDose}_{\text{compartment}} = AR / (RCR_{\text{compartment}} - \text{PEC Reg}_{\text{compartment}} / \text{PNEC}_{\text{compartment}}) \times (\text{TargetRCR} - \text{PEC Reg}_{\text{compartment}} / \text{PNEC}_{\text{compartment}}) \quad \text{Equation 137}$$

Explanation of symbols

$PNEC_{\text{compartment}}$	Predicted no effect concentration for the environmental compartment		
$AR$	Application rate for co-formulant	[kg.ha <sup>-1</sup> ]	User input
$RCR_{\text{compartment}}$	RCR for the environmental compartment, using the original application rate (AR)	[-]	
$\text{Target RCR}$	RCR target	[-]	Default = 0.90
$\text{PEC Reg}_{\text{compartment}}$	Predicted environmental concentration from the background (PEC <sub>regional</sub> ) for the environmental compartment		
$\text{SafeDose}_{\text{compartment}}$	Application rate at target RCR		

For surface water, sediment and soil compartments the  $PEC_{Reg_{compartment}}$  is calculated using  $PEC_{regional}$  values that have been calculated outside the LET (Equation 138).

$$PEC_{Reg_{compartment}} = PEC_{regional_{compartment}} \quad \text{Equation 138}$$

For aquatic and terrestrial predators, the safe dose is calculated using Equation 139 to Equation 141. Again, the maximum dose acceptable for the most sensitive environmental compartment for the substance assessed is reported as the estimated safe dose.

$$SafeDose_{compartment} = AR / RCR_{local\ concentration} \times TargetRCR_{local\ concentration} \quad \text{Equation 139}$$

Where:

$$RCR_{local\ concentration} = F_{local\ diet} \times PEC_{local_{compartment}} / PNEC_{compartment} - F_{local\ diet} \times PEC_{Background_{compartment}} / PNEC_{compartment} \quad \text{Equation 140}$$

$$TargetRCR_{local\ concentration} = TargetRCR - F_{local\ diet} \times PEC_{Background_{compartment}} / PNEC_{compartment} - F_{regional\ diet} \times PEC_{Reg_{compartment}} / PNEC_{compartment} \quad \text{Equation 141}$$

#### Explanation of symbols

$AR$	Application rate for co-formulant	[kg.ha <sup>-1</sup> ]	User input
$RCR_{local\ concentration}$	Local concentration RCR	[-]	Equation 140
$TargetRCR_{local\ concentration}$	Local concentration RCR target	[-]	Equation 141
$F_{local\ diet}$	Fraction of diet from local scale	[-]	Terrestrial, freshwater and marine water predator = 0.5 Aquatic top predator = 0.1
$PEC_{local_{compartment}}$	Predicted environmental concentration at local scale (local + background concentration) for the environmental compartment		
$PEC_{Background_{compartment}}$	Background predicted environmental concentration at the local scale ( $PEC_{regional}$ ) for the environmental compartment		
$PNEC_{compartment}$	Predicted no effect concentration for the environmental compartment		
$Target\ RCR$	Overall RCR target	[-]	Default = 0.90
$F_{regional\ diet}$	Fraction of diet from regional scale	[-]	Terrestrial, freshwater and marine water predator = 0.5 Aquatic top predator = 0.9

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$PEC_{Reg,compartment}$	Predicted environmental concentration at the regional scale ( $PEC_{regional}$ ) for the environmental compartment
$SafeDose_{compartment}$	Application rate at target RCR

---

For aquatic and terrestrial predators, the  $PEC_{Background,compartment}$  and  $PEC_{Reg,compartment}$  are calculated within the LET using Equation 142 to Equation 152. The derivation of  $PEC_{oral, predator}$  is discussed in more detail in Section 3.6.4.2 and Section 3.6.4.3.2.

Aquatic predator:

$$PEC_{Background,compartment} = PEC_{regional,oral,predator} \quad \text{Equation 142}$$

$$PEC_{Reg,compartment} = PEC_{regional,oral,predator} \quad \text{Equation 143}$$

$$PEC_{regional,oral,predator} = PEC_{regional,sw \text{ or } mw(dissolved)} \times BCF_{fish} \times BMF_1 \quad \text{Equation 144}$$

Marine top predator:

$$PEC_{Background,compartment} = PEC_{regional,oral,toppredator} \quad \text{Equation 145}$$

$$PEC_{Reg,compartment} = PEC_{regional,oral,toppredator} \quad \text{Equation 146}$$

$$PEC_{regional,oral,toppredator} = PEC_{regional,sw \text{ or } mw(dissolved)} \times BCF_{fish} \times BMF_1 \times BMF_2 \quad \text{Equation 147}$$

Terrestrial Predator:

$$PEC_{Background,compartment} = PEC_{regional,oral,predator} \quad \text{Equation 148}$$

For the calculation of background exposure of terrestrial predators at the local scale (Equation 148), the  $Regional_{porewater}$  is calculated directly from the regional PEC in agricultural soil (Equation 149).

$$Regional_{porewater} = PEC_{regional,agric.soil} \times RHO_{soil} / (K_{soil-water} \times 1000) \quad \text{Equation 149}$$

$$PEC_{Reg,compartment} = PEC_{regional,oral,predator} \quad \text{Equation 150}$$

For the calculation of exposure of terrestrial predators at the regional scale (Equation 150) the  $Regional_{porewater}$  is taken directly as the regional PEC in porewater of agricultural soil (Equation 151).

$$Regional_{porewater} = PEC_{regional,agric.soil,porewater} \quad \text{Equation 151}$$

$$PEC_{oral,predator} = (BCF_{earthworm} \times Regional_{porewater} + Regional_{agric.soil} \times F_{gut} \times CONV_{soil}) / (1 + F_{gut} \times CONV_{soil}) \quad \text{Equation 152}$$

For humans via the environment where General Population DNELs for both inhalation and oral routes are available, the safe dose is calculated using Equation 153.

$$SafeDose = ((TargetRCR - \sum RegionalRCR_i) / \sum LocalRCR_i) \times AR \quad \text{Equation 153}$$

$i \in \{inhalation, drinking\ water, treated\ crops, milk, meat, fish\}$

## Explanation of symbols

<i>Target RCR</i>	RCR target	[-]	Default = 0.90
<i>RegionalRCR<sub>i</sub></i>	Regional RCR via route i	[-]	Equation 156 or Equation 157, Equation 158, Equation 159, Equation 161, Equation 163
<i>LocalRCR<sub>i</sub></i>	Local RCR via route i	[-]	Equation 164 or Equation 165, Equation 166, Equation 167, Equation 168, Equation 171, Equation 173
<i>AR</i>	Application rate for co-formulant	[kg.ha <sup>-1</sup> ]	User Input
<i>SafeDose</i>	Application rate at target RCR	[kg.ha <sup>-1</sup> ]	

If only the General Population DNEL for inhalation is available (i.e., no General Population DNEL for the oral route), the safe dose is calculated using Equation 154.

$$\text{SafeDose} = (\text{TargetRCR} - \text{RegionalRCR}_{\text{inhalation}}) / \text{LocalRCR}_{\text{inhalation}} \times \text{AR} \quad \text{Equation 154}$$

## Explanation of symbols

<i>Target RCR</i>	RCR target	[-]	Default = 0.90
<i>RegionalRCR<sub>inhalation</sub></i>	Regional RCR via inhalation	[-]	Equation 156 or Equation 157
<i>LocalRCR<sub>inhalation</sub></i>	Local RCR via inhalation	[-]	Equation 165
<i>AR</i>	Application rate for co-formulant	[kg.ha <sup>-1</sup> ]	User Input
<i>SafeDose</i>	Application rate at target RCR	[kg.ha <sup>-1</sup> ]	

If only the General Population DNEL for the oral route is available (i.e., no General Population DNEL for inhalation), the safe dose is calculated using Equation 155.

$$\text{SafeDose} = ((\text{TargetRCR} - \sum \text{RegionalRCR}_i) / \sum \text{LocalRCR}_i) \times \text{AR} \quad \text{Equation 155}$$

$i \in \{\text{inhalation, drinking water, treated crops, milk, meat, fish}\}$

## Explanation of symbols

<i>Target RCR</i>	RCR target	[-]	Default = 0.90
<i>RegionalRCR<sub>i</sub></i>	Regional RCR via route i	[-]	Equation 158, Equation 159, Equation 161, Equation 163



$LocalRCR_i$	Local RCR via route i	[-]	Equation 166, Equation 167, Equation 168, Equation 171, Equation 173
$AR$	Application rate for co-formulant	[kg.ha <sup>-1</sup> ]	User Input
$SafeDose$	Application rate at target RCR	[kg.ha <sup>-1</sup> ]	

For the safe dose calculation, the regional RCRs for man via the environment are calculated. If the General Population DNEL for inhalation is in mg/m<sup>3</sup>, the regional RCR<sub>inhalation</sub> is calculated as:

$$Regional\ RCR_{inhalation} = PEC_{regional\ air} / DNEL_{inhalation} \quad \text{Equation 156}$$

#### Explanation of symbols

$PEC_{regional\ air}$	Regional PEC in air	[mg.m <sup>-3</sup> ]	Input (calculated outside LET)
$DNEL_{inhalation}$	General population, systemic effects, long term inhalation DNEL	[mg.m <sup>-3</sup> ]	User input
$Regional\ RCR_{inhalation}$	Regional RCR for inhalation	[-]	

If the General Population DNEL for inhalation is in mg/kg bw/day, the regional RCR<sub>inhalation</sub> is calculated:

$$Regional\ RCR_{inhalation} = PEC_{regional\ air} \times F_{resp} \times IH_{air} / BW \times BIO_{inh} / BIO_{oral} / DNEL_{inhalation} \quad \text{Equation 157}$$

#### Explanation of symbols

$PEC_{regional\ air}$	Regional PEC in air	[mg.m <sup>-3</sup> ]	Input (calculated outside LET)
$F_{resp}$	Respirable fraction of inhaled substance	[-]	1
$IH_{air}$	Daily intake of air	[m <sup>3</sup> .d <sup>-1</sup> ]	20
$BW$	Bodyweight	[kg]	60
$BIO_{inh}$	Bioavailability by inhalation	[-]	1
$BIO_{oral}$	Bioavailability by oral route	[-]	1
$DNEL_{inhalation}$	General population, systemic effects, long term inhalation DNEL	[mg.kg <sup>-1</sup> .d <sup>-1</sup> ]	User input
$Regional\ RCR_{inhalation}$	Regional RCR for inhalation	[-]	

The RegionalRCR<sub>i</sub> includes regional RCRs for drinking water, treated crops, milk, meat and fish. The Regional RCR for drinking water is calculated as:

$$\text{Regional RCR}_{\text{drw}} = 0.5 \times \text{CONC}_{\text{drw,R}} \times \text{IH}_{\text{drw}} / \text{BW} / \text{DNEL}_{\text{oral}} + 0.5 \times \text{CONC}_{\text{drw,R}} \times \text{IH}_{\text{drw}} / \text{BW} / \text{DNEL}_{\text{oral}} \quad \text{Equation 158}$$

## Explanation of symbols

$\text{CONC}_{\text{drw,R}}$	Regional concentration in drinking water	[mg.L <sup>-1</sup> ]	Equation 107
$\text{IH}_{\text{drw}}$	Daily intake of drinking water	[L.d <sup>-1</sup> ]	2
$\text{BW}$	Bodyweight	[kg]	60
$\text{DNEL}_{\text{oral}}$	General population, systemic effects, long term oral DNEL	[mg.kg <sup>-1</sup> .d <sup>-1</sup> ]	User input
$\text{Regional RCR}_{\text{drw}}$	Regional RCR for drinking water	[-]	

As there is no regional contribution to the intake from treated crops, the Regional RCR for treated crops is 0.

The Regional RCR for intake via fish is calculated as:

$$\text{Regional RCR}_{\text{fish}} = \text{BCF}_{\text{fish}} \times \text{PEG}_{\text{regional}_{\text{sw}}} \times 1000000 \times \text{IH}_{\text{fish}} / \text{BW} / \text{DNEL}_{\text{oral}} \quad \text{Equation 159}$$

## Explanation of symbols

$\text{BCF}_{\text{fish}}$	Bioconcentration factor for fish	[m <sup>3</sup> .kg <sub>wwt</sub> <sup>-1</sup> ]	Equation 123
$\text{PEG}_{\text{regional}_{\text{sw}}}$	Regional predicted environmental concentration in surface water	[kg.m <sup>3</sup> ]	Input (calculated outside LET)
$\text{IH}_{\text{fish}}$	Daily intake of fish	[kg <sub>wwt</sub> .d <sup>-1</sup> ]	0.115
$\text{BW}$	Bodyweight	[kg]	60
$\text{DNEL}_{\text{oral}}$	General population, systemic effects, long term oral DNEL	[mg.kg <sup>-1</sup> .d <sup>-1</sup> ]	User input
$\text{Regional RCR}_{\text{fish}}$	Regional RCR for fish intake	[-]	

The Regional PEC for intake via dairy products is calculated using Equation **160** where regional intake from treated crops is zero and the Regional RCR for intake via dairy products is calculated using Equation **161**.

$$\text{Regional PEC}_{\text{milk}} = \text{BAF}_{\text{milk}} \times (\text{IC}_{\text{soil}} \times \text{PEC}_{\text{regional}_{\text{soil}}} + \text{IH}_{\text{air}} \times \text{PEC}_{\text{regional}_{\text{air}}} + \text{IC}_{\text{drw}} \times \text{CONC}_{\text{drw,R}}) \quad \text{Equation 160}$$

## Explanation of symbols

$\text{BAF}_{\text{milk}}$	Bioaccumulation factor for milk	[day.kg <sub>milk</sub> <sup>-1</sup> ]	Table <b>33</b>
$\text{IC}_{\text{soil}}$	Daily intake of soil (wet weight)	[kg <sub>wwt</sub> .day <sup>-1</sup> ]	Equation 116

$PEC_{regional_{soil}}$	Regional PEC in soil	$[mg.kg_{wwt}^{-1}]$	Input (calculated outside LET)
$IH_{air}$	Daily inhalation rate of cattle	$[m^3.day^{-1}]$	122
$PEC_{regional_{air}}$	Regional PEC in air	$[mg.m^{-3}]$	Input (calculated outside LET)
$IC_{drw}$	Daily intake of drinking water for cattle	$[L.day^{-1}]$	55
$CONC_{drw,R}$	Regional concentration in drinking water	$[mg.L^{-1}]$	Equation 107
$Regional\ PEC_{milk}$	Regional concentration in milk	$[mg.kg_{milk}^{-1}]$	

$$Regional\ RCR_{dairy} = Regional\ PEC_{milk} \times IH_{milk} / BW / DNEL_{oral} \quad \text{Equation 161}$$

## Explanation of symbols

$Regional\ PEC_{milk}$	Regional concentration in milk	$[mg.kg_{milk}^{-1}]$	Equation 160
$IH_{milk}$	Daily intake of dairy products	$[kg_{milk}.d^{-1}]$	0.561
$BW$	Bodyweight	$[kg]$	60
$DNEL_{oral}$	General population, systemic effects, long term oral DNEL	$[mg.kg^{-1}.d^{-1}]$	User input
$Regional\ RCR_{dairy}$	Regional RCR for dairy products	$[-]$	

The Regional PEC for intake via meat is calculated using Equation **162** where regional intake from treated crops is zero and the Regional RCR for intake via meat is calculated using Equation **163**.

$$Regional\ PEC_{meat} = BAF_{meat} \times (IC_{soil} \times PEC_{regional_{soil}} + IH_{air} \times PEC_{regional_{air}} + IC_{drw} \times CONC_{drw,R}) \quad \text{Equation 162}$$

## Explanation of symbols

$BAF_{meat}$	Bioaccumulation factor for meat	$[day.kg_{milk}^{-1}]$	Table 34
$IC_{soil}$	Daily intake of soil (wet weight)	$[kg_{wwt}.day^{-1}]$	Equation 116
$PEC_{regional_{soil}}$	Regional PEC in soil	$[mg.kg_{wwt}^{-1}]$	Input (calculated outside LET)
$IH_{air}$	Daily inhalation rate of cattle	$[m^3.day^{-1}]$	122
$PEC_{regional_{air}}$	Regional PEC in air	$[mg.m^{-3}]$	Input (calculated outside LET)
$IC_{drw}$	Daily intake of drinking water for cattle	$[L.day^{-1}]$	55
$CONC_{drw,R}$	Regional concentration in drinking water	$[mg.L^{-1}]$	Equation 107
$Regional\ PEC_{meat}$	Regional concentration in meat	$[mg.kg_{meat}^{-1}]$	

$$Regional\ RCR_{meat} = Regional\ PEC_{meat} \times IH_{meat} / BW / DNEL_{oral} \quad \text{Equation 163}$$

## Explanation of symbols

$Regional\ PEC_{meat}$	Regional concentration in meat	$[mg \cdot kg_{meat}^{-1}]$	Equation 162
$IH_{meat}$	Daily intake of meat	$[kg_{meat} \cdot d^{-1}]$	0.301
$BW$	Bodyweight	$[kg]$	60
$DNEL_{oral}$	General population, systemic effects, long term oral DNEL	$[mg \cdot kg^{-1} \cdot d^{-1}]$	User input
$Regional\ RCR_{meat}$	Regional RCR for meat	$[-]$	

For the safe dose calculation, the local RCRs for man via the environment are calculated. If the General Population DNEL for inhalation is in  $mg/m^3$ , the local  $RCR_{inhalation}$  is calculated as:

$$Local\ RCR_{inhalation} = (C_{daily,air} + PEC_{regional,air}) / DNEL_{inhalation} \quad \text{Equation 164}$$

#### Explanation of symbols

$C_{daily,air}$	Daily concentration in air	$[mg \cdot m^{-3}]$	Equation 99
$PEC_{regional,air}$	Regional PEC in air	$[mg \cdot m^{-3}]$	Input (calculated outside LET)
$DNEL_{inhalation}$	General population, systemic effects, long term inhalation DNEL	$[mg \cdot m^{-3}]$	User input
$Local\ RCR_{inhalation}$	Local RCR for inhalation	$[-]$	

If the General Population DNEL for inhalation is in  $mg/kg\ bw/day$ , the local  $RCR_{inhalation}$  is calculated:

$$Local\ RCR_{inhalation} = (C_{daily,air} + PEC_{regional,air}) \times F_{resp} \times IH_{air} / BW \times BIO_{inh} / BIO_{oral} / DNEL_{inhalation} \quad \text{Equation 165}$$

#### Explanation of symbols

$C_{daily,air}$	Daily concentration in air	$[mg \cdot m^{-3}]$	Equation 99
$PEC_{regional,air}$	Regional PEC in air	$[mg \cdot m^{-3}]$	Input (calculated outside LET)
$F_{resp}$	Respirable fraction of inhaled substance	$[-]$	1
$IH_{air}$	Daily intake of air	$[m^3 \cdot d^{-1}]$	20
$BW$	Bodyweight	$[kg]$	60
$BIO_{inh}$	Bioavailability by inhalation	$[-]$	1
$BIO_{oral}$	Bioavailability by oral route	$[-]$	1
$DNEL_{inhalation}$	General population, systemic effects, long term inhalation DNEL	$[mg \cdot kg^{-1} \cdot d^{-1}]$	User input
$Local\ RCR_{inhalation}$	Local RCR for inhalation	$[-]$	

The  $LocalRCR_i$  includes Local RCRs for drinking water, treated crops, milk, meat and fish. The Local RCR for drinking water is calculated as:

$$\text{LocalRCR}_{\text{drw}} = 0.5 \times \text{CONC}_{\text{drw,L}} \times \text{IH}_{\text{drw}} / \text{BW} / \text{DNEL}_{\text{oral}} + 0.5 \times \text{CONC}_{\text{drw,R}} \times \text{IH}_{\text{drw}} / \text{BW} / \text{DNEL}_{\text{oral}} \quad \text{Equation 166}$$

## Explanation of symbols

$\text{CONC}_{\text{drw,L}}$	Local concentration in drinking water	[mg.L <sup>-1</sup> ]	Equation 105
$\text{CONC}_{\text{drw,R}}$	Regional concentration in drinking water	[mg.L <sup>-1</sup> ]	Equation 107
$\text{IH}_{\text{drw}}$	Daily intake of drinking water	[L.d <sup>-1</sup> ]	2
$\text{BW}$	Bodyweight	[kg]	60
$\text{DNEL}_{\text{oral}}$	General population, systemic effects, long term oral DNEL	[mg.kg <sup>-1</sup> .d <sup>-1</sup> ]	User input
$\text{Local RCR}_{\text{drw}}$	Local RCR for drinking water	[-]	

As there is no regional contribution to treated crops, the Local RCR for treated crops is:

$$\text{Local RCR}_{\text{crop}} = \text{DOSE}_{\text{crop}} / \text{DNEL}_{\text{oral}} \quad \text{Equation 167}$$

## Explanation of symbols

$\text{DOSE}_{\text{crop}}$	Daily dose via crops	[mg.kg <sup>-1</sup> .bw <sup>-1</sup> ]	Equation 112
$\text{DNEL}_{\text{oral}}$	General population, systemic effects, long term oral DNEL	[mg.kg <sup>-1</sup> .d <sup>-1</sup> ]	User input
$\text{Local RCR}_{\text{crop}}$	Local RCR for crops	[-]	

The Local RCR for intake via fish is calculated as:

$$\text{Local RCR}_{\text{fish}} = \text{BCF}_{\text{fish}} \times \text{C}_{\text{local,sw,HvE,fish}} \times 1000000 \times \text{IH}_{\text{fish}} / \text{BW} / \text{DNEL}_{\text{oral}} \quad \text{Equation 168}$$

## Explanation of symbols

$\text{BCF}_{\text{fish}}$	Bioconcentration factor for fish	[m <sup>3</sup> .kg <sub>wwt</sub> <sup>-1</sup> ]	Equation 123
$\text{C}_{\text{local,sw,HvE,fish}}$	21 day time weighted average in surface water	[µg.L <sup>-1</sup> ]	Equation 78
$\text{IH}_{\text{fish}}$	Daily intake of fish	[kg <sub>wwt</sub> .d <sup>-1</sup> ]	0.115
$\text{BW}$	Bodyweight	[kg]	60
$\text{DNEL}_{\text{oral}}$	General population, systemic effects, long term oral DNEL	[mg.kg <sup>-1</sup> .d <sup>-1</sup> ]	User input
$\text{Local RCR}_{\text{fish}}$	Local RCR for fish intake	[-]	

The Local PEC for intake via dairy products is calculated using Equation 169 and the Local RCR for intake via dairy products is calculated using Equation 171.

$$\text{Local PEC}_{\text{milk}} = \text{BAF}_{\text{milk}} \times (\text{IC}_{\text{grass}} \times \text{C}_{\text{crop,fodder}} + \text{IC}_{\text{soil}} \times \text{TWAC}_{\text{soil}(180\text{d})} + \text{IH}_{\text{air}} \times \text{C}_{\text{field,air,24h}} \times 1000000 + \text{IC}_{\text{drw}} \times \text{Local}_{\text{drw}}) \quad \text{Equation 169}$$

## Explanation of symbols

$BAF_{milk}$	Bioaccumulation factor for milk	$[\text{day} \cdot \text{kg}_{\text{milk}}^{-1}]$	Table 33
$IC_{grass}$	Daily intake of grass (wet weight)	$[\text{kg}_{\text{wwt}} \cdot \text{day}^{-1}]$	Equation 114
$C_{crop, fodder}$	Concentration in fodder crops	$[\text{mg} \cdot \text{kg}_{\text{wwt}}^{-1}]$	Equation 113
$IC_{soil}$	Daily intake of soil (wet weight)	$[\text{kg}_{\text{wwt}} \cdot \text{day}^{-1}]$	Equation 116
$TWAC_{soil(180d)}$	Local concentration in soil (wet weight) as a 180d time weighted average	$[\text{mg} \cdot \text{kg}_{\text{wwt}}^{-1}]$	Equation 36
$IH_{air}$	Daily inhalation rate of cattle	$[\text{m}^3 \cdot \text{day}^{-1}]$	122
$C_{field, air, 24 h}$	24 hour averaged concentration at 10 metres downwind of field	$[\text{kg} \cdot \text{m}^{-3}]$	Equation 98
$IC_{drw}$	Daily intake of drinking water for cattle	$[\text{L} \cdot \text{day}^{-1}]$	55
$Local_{drw}$	Local concentration in drinking water	$[\text{mg} \cdot \text{L}^{-1}]$	Equation 170
$Local PEC_{milk}$	Local concentration in milk	$[\text{mg} \cdot \text{kg}_{\text{milk}}^{-1}]$	

If  $CONC_{drw, L} = \text{Groundwater}$ , then:  $Local_{drw} = PEC_{local, gw\_dw} + PEC_{regional, porewater}$  Equation 170

If  $CONC_{drw, L} = \text{Surfacewater}$ , then:  $Local_{drw} = PEC_{local, sw\_dw}$

## Explanation of symbols

$CONC_{drw, L}$	Local concentration in drinking water	$[\text{mg} \cdot \text{L}^{-1}]$	Equation 105
$PEC_{local, gw\_dw}$	Predicted environmental concentration in soil porewater (drinking water)	$[\text{mg} \cdot \text{L}^{-1}]$	Equation 102
$PEC_{regional, porewater}$	Regional PEC in porewater	$[\text{mg} \cdot \text{L}^{-1}]$	Input (calculated outside LET)
$PEC_{local, sw\_dw}$	Predicted environmental concentration in surface water (drinking water)	$[\text{mg} \cdot \text{L}^{-1}]$	Equation 103
$Local_{drw}$	Local concentration in drinking water	$[\text{mg} \cdot \text{L}^{-1}]$	

$Local RCR_{dairy} = Local PEC_{milk} \times IH_{milk} / BW / DNEL_{oral}$  Equation 171

## Explanation of symbols

$Local PEC_{milk}$	Local concentration in milk	$[\text{mg} \cdot \text{kg}_{\text{milk}}^{-1}]$	Equation 169
$IH_{milk}$	Daily intake of dairy products	$[\text{kg}_{\text{milk}} \cdot \text{d}^{-1}]$	0.561
$BW$	Bodyweight	$[\text{kg}]$	60
$DNEL_{oral}$	General population, systemic effects, long term oral DNEL	$[\text{mg} \cdot \text{kg}^{-1} \cdot \text{d}^{-1}]$	User input
$Local RCR_{dairy}$	Local RCR for dairy products	$[-]$	

The Local PEC for intake via meat is calculated using Equation 172 and the Local RCR for intake via meat is calculated using Equation 173.

$$\text{Local PEC}_{\text{meat}} = \text{BAF}_{\text{meat}} \times (\text{IC}_{\text{grass}} \times \text{C}_{\text{crop}} + \text{IC}_{\text{soil}} \times \text{TWAC}_{\text{soil}(180\text{d})}) + \text{IH}_{\text{air}} \times \text{C}_{\text{field,air,24h}} \times 1000000 + \text{IC}_{\text{drw}} \times \text{Local}_{\text{drw}} \quad \text{Equation 172}$$

## Explanation of symbols

$\text{BAF}_{\text{meat}}$	Bioaccumulation factor for meat	$[\text{day} \cdot \text{kg}_{\text{milk}}^{-1}]$	Table 34
$\text{IC}_{\text{grass}}$	Daily intake of grass (wet weight)	$[\text{kg}_{\text{wwt}} \cdot \text{day}^{-1}]$	Equation 114
$\text{C}_{\text{crop}}$	Concentration in fodder crops	$[\text{mg} \cdot \text{kg}_{\text{wwt}}^{-1}]$	Equation 113
$\text{IC}_{\text{soil}}$	Daily intake of soil (wet weight)	$[\text{kg}_{\text{wwt}} \cdot \text{day}^{-1}]$	Equation 116
$\text{TWAC}_{\text{soil}(180\text{d})}$	Local concentration in soil (wet weight) as a 180d time weighted average	$[\text{mg} \cdot \text{kg}_{\text{wwt}}^{-1}]$	Equation 36
$\text{IH}_{\text{air}}$	Daily inhalation rate of cattle	$[\text{m}^3 \cdot \text{day}^{-1}]$	122
$\text{C}_{\text{field,air,24 h}}$	24 hour averaged concentration at 10 metres downwind of field	$[\text{kg} \cdot \text{m}^{-3}]$	Equation 98
$\text{IC}_{\text{drw}}$	Daily intake of drinking water for cattle	$[\text{L} \cdot \text{day}^{-1}]$	55
$\text{Local}_{\text{drw}}$	Local concentration in drinking water	$[\text{mg} \cdot \text{L}^{-1}]$	Equation 170
$\text{Local PEC}_{\text{meat}}$	Local concentration in meat	$[\text{mg} \cdot \text{kg}_{\text{meat}}^{-1}]$	

$$\text{Local RCR}_{\text{meat}} = \text{Local PEC}_{\text{meat}} \times \text{IH}_{\text{meat}} / \text{BW} / \text{DNEL}_{\text{oral}} \quad \text{Equation 173}$$

## Explanation of symbols

$\text{Local PEC}_{\text{meat}}$	Local concentration in meat	$[\text{mg} \cdot \text{kg}_{\text{meat}}^{-1}]$	Equation 172
$\text{IH}_{\text{meat}}$	Daily intake of meat	$[\text{kg}_{\text{meat}} \cdot \text{d}^{-1}]$	0.301
$\text{BW}$	Bodyweight	$[\text{kg}]$	60
$\text{DNEL}_{\text{oral}}$	General population, systemic effects, long term oral DNEL	$[\text{mg} \cdot \text{kg}^{-1} \cdot \text{d}^{-1}]$	User input
$\text{Local RCR}_{\text{meat}}$	Local RCR for meat	$[-]$	

### 3.7 Environmental regional model: CLE SpERCs

It is considered that the existing Environmental Release Categories (ERCs) given in ECHA guidance R.12 (2015) are not appropriate for estimating exposure at the regional scale associated with co-formulant use in plant protection products.

Therefore, two Specific ERCs (SpERCs) have been developed by CropLife Europe to allow suppliers to calculate regional exposure to co-formulants. This can be done using a SpERC upload file within CHESAR or by transferring the relevant release factors into ECETOC TRA or EUSES.

#### 3.7.1 Scope of the CLE SpERCs

The CLE SpERCs are only intended for use in estimating the contribution of co-formulants at the regional scale and they are to be used in combination with the LET.

It is proposed that the CLE SpERCs can be used for both indoor and outdoor uses of plant protection products, since the parameterisation represents the worst-case that 100% of the substance is released into the environment during its use (emissions to the environment from covered cropping situations might be expected to be lower).

The CLE SpERCs only cover the application stage (i.e., use of the formulated plant protection product and the residues remaining in the environment due to application). Formulation of crop protection products at industrial manufacturing sites is not addressed by the CLE SpERCs and should be addressed using the appropriate ERCs, applying additional refinements as necessary.

It should be noted that for wide dispersive uses (including the CLE SpERCs) direct emissions to air and soil are only considered at the regional scale within the EU-TGD model (as implemented in the TRA). Thus, the CLE SpERC facilitates a regional assessment of human exposure via the environment. This is the standard approach within the TRA, since it is considered unrealistic that all dietary components will be obtained from the local environment.

The potential for emissions to surface water from spray drift is taken into account in SpERC 8d.2.v4. Taking into account the “standard environment” for plant protection product drift scenarios, a reasonable worst-case fraction of 0.002 is assumed to enter a surface water body adjacent to a field as a result of spray drift, and this release factor to surface water is considered in the CLE SpERC for spray application of PPP.

### 3.7.2 Tonnage split between the CLE SpERCs

For a liquid substance used as a co-formulant, the concentration which is achievable in a granular formulation can be assumed to be very limited if it is to remain a solid, and thus the majority of the tonnage could be assigned to spray application methods (i.e., SpERC 8d.2.v4).

For substances which are solids, the end use (e.g., application to a crop) could be either in a liquid or granular formulation, and a tonnage split required between the two CLE SpERCs.

Detailed information on the typical functional use of a substance may help, e.g., a substance used as a filler could be mostly assigned to SpERC 8d.1.v4; an anti-freeze could be mostly assigned to SpERC 8d.2.v4. However, it is proposed that both SpERCs should still be considered, in order not to constrain potential niche applications.

In the absence of any other information, a split of 75% to spray (SpERC 8d.2.v4) and 25% to granule (SpERC 8d.1.v4) application methods could be used for a solid substance used as a co-formulant, on the basis that in general the application of PPP as a spray is more frequent than granular application methods.

### 3.7.3 How to use the CLE SpERCs in TRA

The ECETOC Targeted Risk Assessment (TRA) tool can be freely obtained from <http://www.ecetoc.org/tra>. The ECETOC TRA allows the CLE SpERCs to be defined in both ‘manual’ and ‘batch’ mode. However, to use the most recent version of the CLE SpERCs these should be run in the ‘batch’ mode.

In order to run the tool with the CLE SpERC in batch mode it is necessary to select the following options in the relevant “datasheet” column. Please note that daily amount on site and release times per year are populated to run the model, however, the local PECs should not be used in an assessment.

Option	Input range*	Selection
Fraction of tonnage to region	Row 78	0.1
ERC (mandatory in all cases as use descriptor)	Row 80	ERC 8d
Select approach using SPECIFIC RELEASE FRACTIONS	Row 105	TRUE



Daily amount used on site [kg/d]	Row 123	(Tonnage x Fraction of tonnage to region x Fmain source x 1000)/ emission days
Release times per year (d/year)	Row 124	365
Local release fraction to air	Row 125	See CLE SpERC fact sheet
Local release fraction to sewage	Row 126	See CLE SpERC fact sheet
Local release fraction to soil	Row 127	See CLE SpERC fact sheet

\*ECETOC TRA, Version 3.1

The rest of the TRA (including physico-chemical properties and tonnage data) should be parameterised as normal.

### 3.7.4 How to use the CLE SpERCs in CHESAR

ECHA provide a use maps library which includes the use maps, SpERC factsheets, SpERC briefing note, history of changes to the SpERCs as well as the corresponding Chesar files. These can be found here: <https://echa.europa.eu/csr-es-roadmap/use-maps/use-maps-library>. This information is also available on the CLE REACH-IN webpage.

Information is also available on the ECHA website on how to import and use a use map in Chesar 3 and it is recommended to check the ECHA website for the most recent version of the use map and SpERCs.

Chesar also allows the environmental exposure concentrations from the CLE LET to be inputted into a Chesar assessment. This can be added in the relevant environmental contributing scenario:

- Select ‘Add new exposure dataset’ and ‘External tool’ in the ‘Exposure estimates’ section of the environmental contributing scenario
- Select External tool: ‘CLE LET’
- Input Clocal for each environmental compartment as reported in the CLE LET

### 3.7.5 How to use the CLE SpERCs in EUSES

The most recent version 2.2.0 of the European Union System for the Evaluation of Substances (EUSES) tool is freely available from the ECHA webpage via the link:

<https://echa.europa.eu/support/dossier-submission-tools/euses>

This example describes the input of the CLE SpERC emission factors into EUSES, such that the regional background concentration can be calculated, inclusive of the co-formulant contribution arising from plant protection applications. The description of other life cycle steps – manufacture, formulation – and possible uses e.g., paints, cleaners, detergents etc., are out of scope of this example.

Where only a single CLE SpERC is required, it can be entered by adding a single use (e.g., “Use of co-formulants in plant protection products”) in the “Release estimation” category under “Use patterns – Other life cycle steps”. The emission input data should look like the following example:

**Emission input data**

Usage/production title: Use of co-formulants in plant protection products

Use pattern: Tonnes

Industry category: 1 Agricultural chemicals

Use category: 38 Plant protection products, agricultural

Extra details on use category: No extra details necessary

Extra details on use category: No extra details necessary

Scenario choice for biocides: No extra details necessary

Additional scenario information: No extra details necessary

Biocide scenario life cycle steps: ?

Production

Formulation

Industrial use

Private use

Service life

Waste treatment

Private use

Use specific emission scenario

Emission tables: No applicable emission tables

Emission scenario: no special scenario selected/available

OK Cancel Help

The “Private use” box must be ticked, which causes EUSES to treat the co-formulant use in plant protection products as a wide dispersive use, rather than a point source of emission.

Where both CLE SpERCs are required (e.g., a solid substance), a second use must be entered and the two SpERCs differentiated appropriately e.g. “Spray application of plant protection products containing co-formulants” and “Direct application of plant protection products (granules or treated seeds) containing co-formulants to soil”.

The tonnage for the use of the substance as a co-formulant needs to be appropriately defined (see 3.7.2). The fraction of the substance in the formulation is “1”, since the assessment of environmental exposure will be tonnage-based and a fraction of less than 1 will not alter the final exposure estimate. The regional tonnage for the “private use step” should be 10% of the annual tonnage used as a co-formulant in the EU. In the following example, 100 t/year has been assigned to the co-formulant use:

**Emission input data**

Usage/production title: Use of co-formulants in plant protection products

Use pattern: Tonnes

Fraction of tonnage for application: 1 [-] 0

Total of fractions for all applications: 1 [-] 0

Fraction of chemical in formulation: 1 [-] 0

Tonnage of formulated product: 100 [tonnes-yr] 0

Relevant tonnage for application: 100 [tonnes-yr] 0

Regional tonnage of substance: 100 [tonnes-yr] 0

Continental tonnage of substance: 0 [tonnes-yr] 0

Regional tonnage of substance (private use step): 10 [tonnes-yr] 0

Continental tonnage of substance (private use step): 90 [tonnes-yr] 0

OK Cancel Help

The release fractions are defined according to the CLE SpERCs, and are entered in the “Release estimation” category under “Intermediate results” for the “private use” step. For spray applications these fractions are vapour pressure dependent.

The “fraction of the main local source” is set to “zero” because the assessment is done solely for the regional scale. This effectively turns off the local scale assessment within EUSES, and prevents the tonnage assigned to the co-formulant use from incorrectly contributing to local STP emissions.

The “number of emission days” refers to the exposure on the local scale and therefore does not affect the exposure estimate for the regional scale. It was set to “365” in the following example to make clear that wide dispersive use is assessed:

Release fractions and emission days [2 "Use of co-formulants in plant prot...]

Private use

No applicable emission tables

Release fractions

Fraction of tonnage released to air	0	[-]	s
Fraction of tonnage released to wastewater	0	[-]	o
Fraction of tonnage released to surface water	0	[-]	s
Fraction of tonnage released to industrial soil	0	[-]	o
Fraction of tonnage released to agricultural soil	1	[-]	s
Emission fractions determined by special scenario	No		o

Emission days

Fraction of the main local source	0	[-]	o
Number of emission days per year	365	[-]	o
Release to wastewater only	No		o
Emission days determined by special scenario	No		o

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## 5 Appendices

### *Appendix 1: Summary of changes between different versions of the REACH-IN Local Environment Tool (LET)*

The latest version of the CLE REACH-IN Local Environment Tool (LET) v.4.0 reflects the name change of the European Crop Protection Association (ECPA) to CropLife Europe (CLE). The tool has been updated with the following changes:

- The ‘Default’ assessment assumes 10 years of successive applications to soil which is analogous to the EUSES approach which considers successive sewage sludge applications to soil
- The mixing depth used for calculating the rate constant for volatilisation and leaching in soil has been updated to vary with the mixing depth selected at application
- The ‘Refinement Options’ assessment includes an option to select 1 year application to soil
- The emission fractions to soil and air have been updated in line with CLE SpERCs v4.0
- The ‘Refinement Options’ assessment allows direct editing of the emission fractions to soil and air
- Humans via environment assessment for estimating local dietary exposure included with an option to enter DNELs in Input sheet
- In line with the update to the humans via environment assessment, regional PEC in air is an input and can be imported from the ECETOC TRA

The effect of the above changes has been investigated using a number of test substances with varying physical-chemical and environmental fate properties and ecotoxicity and toxicity profiles.

<b>Endpoint</b>	<b>Substance 1</b>	<b>Substance 2</b>	<b>Substance 3</b>	<b>Substance 4</b>	<b>Substance 5</b>
Physical state	Liquid	Solid	Solid	Liquid	Liquid
Molecular weight (g/mol)	99.1	151.2	128.2	199.3	202.3
Water solubility (mg/L)	1000000	1153	31.7	340	429
Vapour pressure (Pa)	32	1.80E-04	7.2	0.11	0.124
Log Kow	-0.46	0.7	3.4	3.44	3.3
Biodegradability classification	Readily degradable	Not biodegradable	Readily biodegradable	Readily biodegradable	Readily biodegradable
PNEC aquatic (mg/L)	0.25	0.004	0.0024	0.028	0.008
<b>Endpoint</b>	<b>Substance 6</b>	<b>Substance 7</b>	<b>Substance 8</b>	<b>Substance 9</b>	<b>Substance 10</b>
Physical state	Liquid	Liquid	Liquid	Solid	Solid
Molecular weight (g/mol)	102.1	74.1	185.2	373.2	691.1
Water solubility (mg/L)	200000	70000	50000	20	0.853
Vapour pressure (Pa)	6	1600	69.8	6.30E-06	1.00E-08
Log Kow	-0.41	1	-0.41	3.83	4.77
Biodegradability classification	Readily biodegradable	Readily biodegradable	Readily biodegradable	Not biodegradable	Readily biodegradable
PNEC aquatic (mg/L)	0.9	0.4	0.073	0.01	0.28

The assessment of these randomly selected test substances with the LET versions 3.1 and 4.0 resulted in similar predicted safe application rates. Slightly lower safe application rates are predicted with version 4.0 for the spray application of two substances. The safe application rates predicted with version 4.0 are slightly higher for a few substances when applied as granules or treated seeds.

	<b>Maximum safe application rate (kg/ha), default assessment, one application</b>			
	<b>LET 3.1</b>	<b>LET 4.0</b>	<b>LET 3.1</b>	<b>LET 4.0</b>
	<b>Spray application</b>	<b>Spray application</b>	<b>Granular application</b>	<b>Granular application</b>
Substance 1	4.3	4.3	0.0716	0.0907
Substance 2	0.00118	0.00116	0.00094	0.00116
Substance 3	0.0413	0.0413	0.0291	0.0291
Substance 4	0.482	0.482	0.281	0.286
Substance 5	0.138	0.138	0.0508	0.052
Substance 6	15.48	15.48	0.241	0.307
Substance 7	6.88	6.88	0.0961	0.187
Substance 8	1.26	1.26	0.015	0.0271
Substance 9	0.0972	0.0965	0.143	0.143
Substance 10	4.82	4.82	17.33	17.33

A comparison of tool versions 2.0 and 3.0 had been conducted previously, using a set of four test substances. This comparison is described below.

**Table A 1: The four test substances used to investigate the effect of changes between ECPA REACH-IN LET v2.0 and v3.0**

<b>Endpoint</b>	<b>Test Substance 1</b>	<b>Test Substance 2</b>	<b>Test Substance 3</b>	<b>Test Substance 4</b>
Molecular weight (g/mol)	101	122	86	363.1
Water solubility (mg/L)	6000	105	0.063	50000
Temperature water solubility was measured (°C)	20	20	20	20
Vapour pressure (Pa)	5000	0.0089	0.0000069	0.0004
Temperature vapour pressure was measured (°C)	20	30	20	20
K <sub>ow</sub> (log value)	0.5	3	3.2	-0.1
Biodegradability classification	Readily biodegradable	Readily biodegradable	Not biodegradable	Readily biodegradable
QSAR for K <sub>oc</sub>	Non hydrophobic	Non hydrophobic	Non hydrophobic	Non hydrophobic
PNEC aquatic (mg/L)	0.5	0.04	0.3	0.6
Formulation type	Spray	Spray	Granule/treated seed	Spray

The four substances summarised in Table A 1 cover a range of physical properties and application scenarios.

Test substance 1 is very volatile and applied in a spray formulation with exposure driven by volatilisation to air during spraying and spray drift onto the adjacent waterbody. Release to soil is expected to be negligible and the calculation of safe application rate is driven by the most sensitive compartment which is surface water.

Test substance 2 is also applied in a spray formulation but the vapour pressure is much lower and release is predicted to soil and surface water (via spray drift and runoff/drainage). Surface water is the most sensitive compartment and drives the calculation of a safe application rate.

Test substance 3 is applied as a granule treatment and no volatilisation or spray drift is assumed. The calculation of safe application rate is driven by soil.

Test substance 4 is applied as a spray and has a relatively low vapour pressure. Exposure is expected to soil and surface water (via spray drift and runoff/drainage) but the soil compartment drives the calculation of a safe application rate.

The four scenarios are also summarised in Table A 2.

**Table A 2: Summary of four test scenarios**

Test Substance	Formulation Type	Initial exposure pathways	Limiting RCR
Test Substance 1	Spray	Spray drift to surface water	Surface water
Test Substance 2	Spray	Spray drift to surface water Runoff/drainage to surface water Fraction applied to soil	Surface water
Test Substance 3	Granule	Direct application to soil Runoff/drainage to surface water	Agricultural soil
Test Substance 4	Spray	Spray drift to surface water Runoff/drainage to surface water Fraction applied to soil	Agricultural soil

It should be noted that these test substances have been developed for testing purposes and do not represent existing co-formulants. The testing approach and the range of test substances selected also do not constitute an in-depth investigation of the effect of changes in version 3.0 compared to version 2.0. The intention is to illustrate the possible differences that may be seen in results between version 2.0 and version 3.0.

## Results

*Target RCR set to 0.90 in ECPA LET v2.0 and ECPA LET v3.0*

Regional PEC's were included in the assessments. The PECs and safe application rates for version 2 and version 3 for each test substance are reported in Table A 3 to Table A 6.

**Table A 3: Summary of results for test substance 1 when v2 and v3 both have a Target RCR of 0.90**

	Test substance 1	
	v2	v3
PEC surface water (mg/L)	0.4500	0.4500
PEC sediment (mg/kg dwt)	0.0590	0.0590
PEC marine water (mg/L)	0.0450	0.0450
PEC marine sediment (mg/kg dwt)	0.0059	0.0059
PEC agricultural soil (mg/kg dwt)	5.59E-05	5.59E-05
PEC aquatic predator (mg/kg wet fish)	0.1190	0.1190
PEC terrestrial predator (mg/kg wet earthworm)	5.42E-06	5.06E-05



PEC marine predator (mg/kg wet fish)	n/a	0.0119
PEC marine top predator (mg/kg wet fish)	n/a	2.39E-03
Safe dose (kg/ha)	8.60	8.60
Target RCR	0.90	0.90

**Table A 4: Summary of results for test substance 2 when v2 and v3 both have a Target RCR of 0.90**

	Test substance 2	
	v2	v3
PEC surface water (mg/L)	0.0360	0.0360
PEC sediment (mg/kg dwt)	0.1320	0.1320
PEC marine water (mg/L)	0.0036	0.0036
PEC marine sediment (mg/kg dwt)	0.0132	0.0132
PEC agricultural soil (mg/kg dwt)	0.2290	0.2280
PEC aquatic predator (mg/kg wet fish)	1.27	1.27
PEC terrestrial predator (mg/kg wet earthworm)	0.0595	0.0591
PEC marine predator (mg/kg wet fish)	n/a	0.1270
PEC marine top predator (mg/kg wet fish)	n/a	0.0255
Safe dose (kg/ha)	0.476	0.476
Target RCR	0.90	0.90

**Table A 5: Summary of results for test substance 3 when v2 and v3 both have a Target RCR of 0.90**

	Test substance 3	
	v2	v3
PEC surface water (mg/L)	0.2000	0.2010
PEC sediment (mg/kg dwt)	0.9850	0.9880
PEC marine water (mg/L)	0.0200	0.0201
PEC marine sediment (mg/kg dwt)	0.0983	0.0986
PEC agricultural soil (mg/kg dwt)	2.64	2.64
PEC aquatic predator (mg/kg wet fish)	10.49	10.54
PEC terrestrial predator (mg/kg wet earthworm)	2.46	2.44
PEC marine predator (mg/kg wet fish)	n/a	1.05
PEC marine top predator (mg/kg wet fish)	n/a	0.213
Safe dose (kg/ha)	1.98	1.99
Target RCR	0.90	0.90

**Table A 6: Summary of results for test substance 4 when v2 and v3 both have a Target RCR of 0.90**

	Test substance 4	
	v2	v3

PEC surface water (mg/L)	0.0330	0.0352
PEC sediment (mg/kg dwt)	0.0032	0.0034
PEC marine water (mg/L)	0.0033	0.0035
PEC marine sediment (mg/kg dwt)	3.17E-04	3.38E-04
PEC agricultural soil (mg/kg dwt)	0.1720	0.1720
PEC aquatic predator (mg/kg wet fish)	0.0027	0.0029
PEC terrestrial predator (mg/kg wet earthworm)	0.0703	0.0626
PEC marine predator (mg/kg wet fish)	n/a	2.89E-04
PEC marine top predator (mg/kg wet fish)	n/a	5.82E-05
Safe dose (kg/ha)	0.224	0.239
Target RCR	0.90	0.90

### ***Conclusion***

Where the ECPA LET v2.0 and v3.0 are run as a 'Default' assessment with the same target RCR some differences were observed. Where soil was the most sensitive compartment and thus used to calculate the safe application rate, a slight increase in the safe application rate was observed in v3.0. This resulted in slightly higher PECs in all environmental compartments except soil and terrestrial predators. Where surface water drove the safe application rate calculation, the safe application rates remained the same between versions. However, where the PEC in agricultural soil and terrestrial predators is calculated, these PECs decreased slightly.

It should be noted that these observations are based on only four test substances and is not an in-depth investigation of changes between ECPA LET v2.0 and ECPA LET v3.0. Other changes, not mentioned here may be encountered (e.g., where substances have a log  $K_{ow}$  of 8 or 9 the PEC freshwater predator is expected to increase by an approximate factor of 3).

## *Appendix 2: Approach for estimating individual crop yields used in humans via environment assessment*

The CLE REACH-IN Local Environment Tool (LET) v4.0 includes a module to conduct a screening assessment of exposure to humans via the environment. This includes crop yield data for estimating intake via crops and estimating intake by meat and milk following consumption of crops by cattle.

The average yields were calculated for 13 representative crops using data obtained from EUROSTAT ([https://appsso.eurostat.ec.europa.eu/nui/show.do?dataset=apro\\_cpsh1&lang=en](https://appsso.eurostat.ec.europa.eu/nui/show.do?dataset=apro_cpsh1&lang=en)) extracted on 07/12/2020. Crops were selected to most closely represent the crop category covered by the assessment (shown in Table A 7). In some cases a crop was selected to represent a wider crop group and the representative crop selected was based on the crop type used for selecting the PRIMO intake values or expert opinion. For the EUROSTAT crop selected, where the crop yield (t/ha) was reported, this was used directly. Where crop yield was not reported by EUROSTAT, it was estimated from harvested production (1000 t) and area (cultivation/harvested/production) (ha). The average crop yield per year (shown in Table A 7) represents an average across 28 EU member states (Belgium, Bulgaria, Czechia, Denmark, Germany, Estonia, Ireland, Greece, Spain, France, Croatia, Italy, Cyprus, Latvia, Lithuania, Luxembourg, Hungary, Malta, Netherlands, Austria, Poland, Portugal, Romania, Slovenia, Slovakia, Finland, Sweden, United Kingdom). The 9 year average (2011-2019) was selected for use in the LET (Table 32).

**Table A 7: Average crop yields (tonnage/ha) for 28 EU member states from 2011 to 2019**

<b>Crops</b>	<b>2011</b>	<b>2012</b>	<b>2013</b>	<b>2014</b>	<b>2015</b>	<b>2016</b>	<b>2017</b>	<b>2018</b>	<b>2019</b>	<b>9 year average</b>
Pome/stone fruit (EUROSTAT crop: Apples)	19.97	17.52	19.67	21.89	22.18	19.11	16.66	23.15	20.49	<b>20.1</b>
Citrus (EUROSTAT crop: Citrus fruits)	22.14	22.03	21.10	22.97	20.84	21.02	20.63	21.84	20.40	<b>21.4</b>
Berries (EUROSTAT crop: Berries (excluding strawberries))	3.88	3.38	3.39	4.01	4.83	4.45	4.79	4.99	4.89	<b>4.3</b>
Table grapes (EUROSTAT crop: Table grapes)	9.72	10.17	10.28	9.32	9.21	9.82	9.19	10.47	10.16	<b>9.8</b>
Cereals (EUROSTAT crop: Common wheat and spelt)	5.12	4.92	5.26	5.69	5.89	5.21	5.56	5.04	5.78	<b>5.4</b>
Pulses (EUROSTAT crop: Fresh peas)	5.64	4.98	5.40	5.52	5.61	5.45	5.20	4.59	5.19	<b>5.3</b>
Oil seeds (EUROSTAT crop: Rape and turnip rape seeds)	2.76	2.74	2.90	3.20	3.09	2.90	3.06	2.79	2.97	<b>2.9</b>
Root vegetables (EUROSTAT crop: Carrots)	41.78	42.33	40.77	42.67	41.18	41.99	41.56	39.99	42.20	<b>41.6</b>
Leafy vegetables (EUROSTAT crop: Lettuces)	22.89	24.01	21.84	22.11	23.77	22.66	23.38	22.95	23.09	<b>23.0</b>

Bulb vegetables (EUROSTAT crop: Onions)	32.81	32.48	31.56	33.45	31.74	30.57	29.07	27.11	29.64	<b>30.9</b>
Tomatoes (EUROSTAT crop: Tomatoes)	62.88	65.48	65.44	63.80	69.67	72.71	72.17	69.79	70.48	<b>68.0</b>
Brassica vegetables (EUROSTAT crop: Brassicas)	32.60	31.95	30.31	30.70	27.44	27.01	27.31	25.82	27.12	<b>28.9</b>
Animal fodder (EUROSTAT crop: average green fodder)	12.62	12.62	12.09	14.03	14.38	16.77	17.06	15.18	17.53	<b>14.7</b>

### *Appendix 3: Approach for estimating crop consumption used in humans via environment assessment*

The CLE REACH-IN Local Environment Tool (LET) v4.0 includes a module to conduct a screening assessment of exposure to humans via the environment. This includes food consumption data for individual crop categories for estimating intake via treated crops. The food intake values selected represent the maximum average food consumption for representative crop categories across adult diets in 16 member states and 6 GEMS/Food Cluster diets relevant for the EU Member States (i.e., cluster diet G06, G07, G08, G10, G11 and G15) used in the EFSA PRIMo model for chronic exposure assessments. For each crop category, a representative crop (or PRIMo food product) was selected based on the food product that had the highest average food consumption across the most member state and GEMS/Food Cluster diets considered. The food product selected for each crop category are reported in Table A 8.

The maximum average food consumption (g/kg bw/d) across the member state and GEMS/Food Cluster diets for each crop was selected and multiplied by the corresponding mean bodyweight (kg) for that data set to calculate the daily average consumption (kg/day) per crop (Table A 9).

**Table A 8: Average consumption (g/kg bw/d) data for adult member state and GEMS/Food Cluster diets taken from EFSA PRIMo v3 (bold indicates maximum intake selected to represent crop category)**

Crops (EFSA PRIMo food product)	DK	ES	FI	FR	IE	IT	LT	NL	PL	PT	RO	SE	UK	UK*	DE	DE**	GEMS Food G06	GEMS Food G07	GEMS Food G08	GEMS Food G10	GEMS Food G11	GEMS Food G15	Maximum adult intake
Pome/stone fruit (apples)	0.96	0.77	0.58	0.77	0.71	0.79	1.87	1.46	2.04	1.05	1.42	1.05	0.41	0.59	2.43	<b>2.58</b>	0.92	1.02	1.21	0.75	1.55	1.09	<b>2.58</b>
Citrus (oranges)	0.14	1.29	0.41	0.59	1.04	0.37	0.07	1.01	0.02	0.61	0.28	0.75	0.56	0.87	1.56	<b>1.91</b>	1.00	1.39	0.46	1.13	0.73	0.67	<b>1.91</b>
Berries (strawberries)	0.07	0.06	0.14	0.12	<b>0.18</b>	0.05	0.04	0.09	0.02	0.04	0.05	0.17	0.05	0.07	0.11	0.12	0.04	0.07	0.09	0.11	0.10	0.06	<b>0.18</b>
Table grapes (table grapes)	0.17	0.04	0.08	0.11	0.26	0.13	0.01	0.25	0.32	0.28	0.18	n.d.	0.05	0.08	0.26	0.30	<b>1.05</b>	0.33	0.33	0.30	0.42	0.34	<b>1.05</b>
Cereals (wheat)	1.12	2.35	0.32	2.22	2.30	4.14	1.05	1.93	n.d.	3.92	5.07	3.20	1.68	2.05	1.88	2.15	<b>7.23</b>	4.22	4.08	3.92	3.61	4.54	<b>7.23</b>
Pulses (beans)	0.01	0.05	0.01	0.12	0.12	0.06	n.d.	0.04	0.03	0.17	0.12	n.d.	0.22	<b>0.36</b>	0.02	0.01	0.12	0.03	0.03	0.09	0.02	0.06	<b>0.36</b>
Oilseeds (rapeseeds/canola seeds)	n.d.	n.d.	0.00	0.00	n.d.	n.d.	n.d.	0.26	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.01	0.01	0.03	<b>0.54</b>	0.33	0.26	n.d.	0.20	<b>0.54</b>
Root vegetables (potatoes)	1.27	0.93	1.18	0.73	2.29	0.60	3.17	2.43	3.44	<b>5.33</b>	3.73	4.17	1.40	1.37	1.23	1.10	2.00	3.75	3.90	2.96	3.91	3.56	<b>5.33</b>
Leafy vegetables (lettuce)	0.09	0.54	0.14	0.18	0.09	<b>0.56</b>	0.06	0.19	0.01	0.11	n.d.	0.40	0.12	0.14	0.12	0.14	0.16	0.27	0.28	0.42	0.21	0.11	<b>0.56</b>
Bulb vegetables (onions)	0.15	0.20	0.15	0.13	0.15	0.10	n.d.	0.22	0.33	0.35	0.75	0.45	0.15	0.23	0.11	0.10	<b>0.76</b>	0.35	0.51	0.58	0.18	0.52	<b>0.76</b>
Tomatoes	0.52	0.78	0.56	0.46	0.40	1.16	0.62	0.42	0.88	0.90	1.93	0.77	0.44	0.62	0.66	0.74	<b>3.58</b>	1.08	1.14	1.37	0.91	1.19	<b>3.58</b>
Brassica vegetables (cauliflower)	0.04	0.06	0.04	0.14	0.16	0.05	n.d.	<b>0.19</b>	0.09	0.02	0.03	0.08	0.06	0.11	0.15	0.15	0.03	0.09	0.08	0.05	0.09	0.05	<b>0.19</b>

\*UK vegetarian, \*\* DE women 14-50 years, n.d. Average consumption data not reported for member state/GEMS/Food Cluster

**Table A 9: Daily average consumption (kg/d) for 12 crop categories (adult food intake and corresponding average body weights taken from EFSA PRIMo v3**

Crops (EFSA PRIMo food product)	Maximum adult intake (g/kg bw/d)	Average body weight (kg)	Maximum daily crop consumption (kg/d)
Pome/stone fruit (apples)	2.58	76.4	0.1968
Citrus (oranges)	1.91	76.4	0.1461
Berries (strawberries)	0.18	75.2	0.0135
Table grapes (table grapes)	1.05	60.0	0.0631
Cereals (wheat)	7.23	60.0	0.4341
Pulses (beans)	0.36	66.7	0.0238
Oilseeds (rapeseeds/canola seeds)	0.54	60.0	0.0327
Root vegetables (potatoes)	5.33	60.0	0.3200
Leafy vegetables (lettuce)	0.56	66.5	0.0371
Bulb vegetables (onions)	0.76	60.0	0.0454
Tomatoes	3.58	60.0	0.2148
Brassica vegetables (cauliflower)	0.19	65.8	0.0126