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

The REACH-IN Project

26 August 2021

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Sector Specific Terminology and Abbreviations

Plant Protection Product Terminology	REACH Equivalent Terminology / Clarification
AI	Active ingredient
PPP	Plant protection product
CPP	Crop protection products
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 is making the CLE OWB and LET available for users to aid them in the human and local scale environmental risk assessment of 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 t/year. For substances meeting the criteria for classification under Regulation (EC) No. 1272/2008 (CLP), a quantitative 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/pre-market-resources/reach-in-registration-evaluation-authorisation-and-restriction-of-chemicals/).

In the case of professional workers (i.e. farmers) and consumers, an exposure modelling tool (OWB) has been developed to assess the potential exposure to co-formulants arising from plant protection uses. CLE OWB allows the user 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 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 outdated versions of the SpERCs), 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 impacts.

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 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 co-formulants.

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.

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 on the basis of 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 ERCs are not appropriate for 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. While not necessarily covering all possible application methods, the four GES are considered to cover the most common methods.

No.	Identified Use	Use Descriptors
1	Use as a co-formulant in plant protection products, spray applications by professionals	PW, SU1, PROC 8a, PROC 11, CLE SpERC 8d.2.v4
2	Use as a co-formulant in plant protection products, seed and granular applications by professionals	PW, SU1, PROC 8a, PROC 8b, CLE SpERC 8d.1.v4
3	Use as a co-formulant in plant protection products, spray applications by consumers	C, PC27, CLE SpERC 8d.2.v4
4	Use as a co-formulant in plant protection products, seed and granular applications by consumers	C, PC27, CLE SpERC 8d.1.v2

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), consumers and the environment.

Professional Uses – Generic Exposure Scenario 1		
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, CLE SpERC 8d.2.v4
Environment CS 1	CLE SpERC 8d.2.v4	Spray application of plant protection products containing co-formulants (indoor or outdoor)
Worker CS 2	PROC 8a	Mixing and loading of plant protection products into delivery equipment
Worker CS 3	PROC 11	Delivery and dispersion of plant protection products

Professional Uses – Generic Exposure Scenario 2		
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, CLE SpERC 8d.1.v4
Environment CS 1	CLE SpERC 8d.1.v4	Direct application of plant protection products (granules or treated seeds) containing co-formulants to soil (indoor or outdoor)
Worker CS 2	PROC 8a	Mixing and loading of plant protection products into seed treatment or delivery equipment
Worker CS 3	PROC 8b	Transfer of treated seeds from batch treater into bags
Worker CS 4	PROC 8a	Delivery and dispersion of agrochemical plant protection products or treated seeds

Consumer Uses – Generic Exposure Scenario 3		
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	Spray application of plant protection products containing co-formulants (indoor or outdoor)
Consumer CS 2	PC27	Spray application of agrochemical plant protection products

Consumer Uses – Generic Exposure Scenario 4		
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	Direct application of plant protection products (granules or treated seeds) containing co-formulants to soil (indoor or outdoor)
Consumer CS 2	PC27	Manual spreading of granular plant protection products or treated seeds

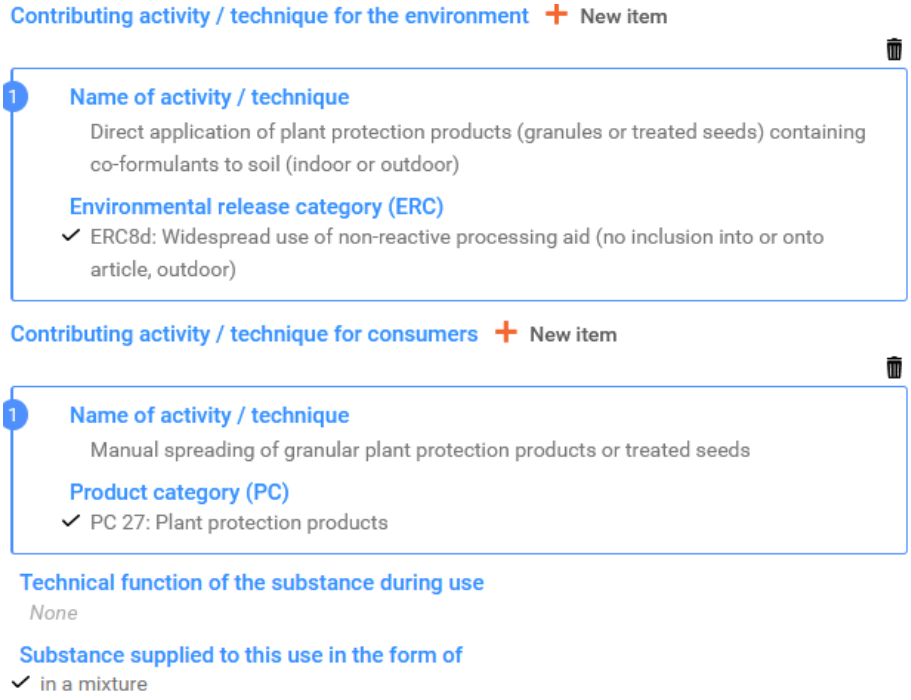
Further activities related to smaller scale application methods, such as painting, fogging, dusting, and dipping, while not included above, are likely to fall either within the scope of generic exposure scenarios describing the use of substances in mixtures and formulations, and as such may not warrant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

1.2.1 Use Descriptor Entry in IUCLID 6

The following examples are for Use Descriptor entry in IUCLID 6 (version 5.1.2) Section 3.5.

Use by Professional Workers

Consumers Uses



1.2.2 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).

1.3 Link from Generic Exposure Scenarios to REACH-IN Tools

In principle many different Tier 1, or higher, models could be used to generate exposure estimates for the above activities. 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) linked to the above scenarios suitable for use in REACH risk assessments. The use of these tools 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 above 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.

1.3.1 Identified Use / PPP GES1 – Use as a co-formulant in plant protection products, spray applications by professionals

ERC8d: CLE SpERC 8d.2.v4 - Spray application of plant protection products containing co-formulants

The CLE spray application SpERC (8d.2.v4) considers vapour-pressure dependent direct emissions to soil and/or air, which for wide dispersive uses are considered only at the regional scale. Background information on the development of the SpERC has been published (Dobe *et al.* 2020). The latest CLE SpERC 8d.2.v4 is available as a SpERC factsheet and as a Chesar file on the webpages of CropLife Europe and ECHA. The SpERC has been implemented in ECETOC TRA, however, the latest version 3.1 of TRA still uses version 2 of the CLE SpERCs. If the regional environmental risk assessment is performed with ECETOC TRA, the release factors need to be changed manually according to the latest SpERC factsheet to calculate the regional environmental releases from the co-formulant use correctly.

The SpERC is not intended to provide a definitive estimate of environmental exposure at the local scale. It must be combined with use of the LET.

The CLE SpERC, when selected in ECETOC TRA or Chesar, is used to estimate the contribution to the regional background concentrations ($PEC_{regional}$) from the use of PPP by spraying; any local scale PECs calculated in ECETOC TRA or Chesar should be disregarded. The emission factors encoded in the SpERC can also be transferred to other tools to calculate the regional background PECs, e.g. EUSES.

Following import of the $PEC_{regional}$ into the LET, the spraying scenario can be run to estimate local PECs.

PROC 8a: Loading of plant protection products into delivery equipment

Description of the activities and technical processes: 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.

PROC 11: Spray application of agrochemical plant protection products

Description of the activities and technical processes: 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.

1.3.2 Identified Use / PPP GES2 – Use as a co-formulant in plant protection products, seed and granular applications by professionals

ERC8d: CLE SpERC 8d.1.v4 - Direct application of plant protection products (granules or treated seeds) containing co-formulants to soil (indoor or outdoor)

The CLE treated seed/granular application SpERC (8d.1.v4) considers direct emissions to soil, which for wide dispersive uses are considered only at the regional scale. Background information on the development of the SpERC has been published (Dobe *et al.* 2020). The latest CLE SpERC 8d.1.v4 is available as a SpERC factsheet and as a Chesar file on the webpages of CropLife Europe and ECHA. The SpERC has been implemented in ECETOC TRA, however, the latest version 3.1 of TRA still uses version 2 of the CLE SpERCs. If the regional environmental risk assessment is performed with ECETOC TRA, the release factors need to be changed manually according to the latest SpERC factsheet to calculate the regional environmental releases from the co-formulant use correctly.

The SpERC is not intended to provide a definitive estimate of environmental exposure at the local scale. It must be combined with use of the LET.

The CLE SpERC, when selected in ECETOC TRA or Chesar, is used to estimate the contribution to the regional background concentrations ($PEC_{regional}$) from the use of treated seeds/granular PPP; any local scale PECs calculated in ECETOC TRA or Chesar should be disregarded. The emission factors encoded in the SpERC can also be transferred to other tools to calculate the regional background PECs, e.g. EUSES.

Following import of the $PEC_{regional}$ into the LET, the treated seed/granular scenario can be run to estimate local PECs.

PROC 8a: Loading of plant protection products into delivery equipment

Description of the activities and technical processes: 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.

PROC 8a: Delivery and dispersion of agrochemical plant protection products

Description of the activities and technical processes: The delivery and dispersion of treated seeds and granular PPPs 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.

1.3.3 Identified use / PPP GES3 – Use as a co-formulant in plant protection products, spray applications by consumers

ERC8d: CLE SpERC 8d.2.v4 - Spray application of plant protection products containing co-formulants

The CLE spray application SpERC (8d.2.v4) considers vapour-pressure dependent direct emissions to soil and/or air, which for wide dispersive uses are considered only at the regional scale. Background information on the development of the SpERC has been published (Dobe *et al.* 2020). The latest CLE SpERC 8d.2.v4 is available as a SpERC factsheet and as a Chesar file on the webpages of CropLife Europe and ECHA. The SpERC has been implemented in ECETOC TRA, however, the latest version 3.1 of TRA still uses version 2 of the CLE SpERCs. If the regional environmental risk assessment is performed with ECETOC TRA, the release factors need to be changed manually according to the latest SpERC factsheet to calculate the regional environmental releases from the co-formulant use correctly.

The SpERC is not intended to provide a definitive estimate of environmental exposure at the local scale. It must be combined with use of the LET.

The CLE SpERC, when selected in ECETOC TRA or Chesar, is used to estimate the contribution to the regional background concentrations ($PEC_{regional}$) from the use of PPP by spraying; any local scale PECs calculated in ECETOC TRA or Chesar should be disregarded. The emission factors encoded in the SpERC can also be transferred to other tools to calculate the regional background PECs, e.g. EUSES.

Following import of the $PEC_{regional}$ into the LET, the spraying scenario can be run to estimate local PECs.

PC 27: Loading of plant protection products into delivery equipment

Description of the activities and technical processes: The transfer (and inherent diluting and mixing) of solid and liquid PPP which occurs during loading of hand-held spray equipment.

The OWB calculates exposures varying all the variable exposure determinants, as in the professional scenario, 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 exposure value for mixing and loading activities in the contributing scenario for risk assessment.

PC 27: Spray application of agrochemical plant protection products

Description of the activities and technical processes: The spray application of PPP using hand-held spray equipment for high-level targets.

The OWB calculates exposures varying all the variable exposure determinants, as in the professional scenario, 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 exposure value for spraying activities in the contributing scenario for risk assessment.

1.3.4 Identified Use / PPP GES4 – Use as a co-formulant in plant protection products, seed and granular applications by consumers

ERC8d: CLE SpERC 8d.1.v4 - Direct application of plant protection products (granules or treated seeds) containing co-formulants to soil (indoor or outdoor)

The CLE treated seed/granular application SpERC (8d.1.v4) considers direct emissions to soil, which for wide dispersive uses are considered only at the regional scale. Background information on the development of the SpERC has been published (Dobe *et al.* 2020). The latest CLE SpERC 8d.1.v4 is available as a SpERC factsheet and as a Chesar file on the webpages of CropLife Europe and ECHA. The SpERC has been implemented in ECETOC TRA, however, the latest version 3.1 of TRA still uses version 2 of the CLE SpERCs. If the regional environmental risk assessment is performed with ECETOC TRA, the release factors need to be changed manually according to the latest SpERC factsheet to calculate the regional environmental releases from the co-formulant use correctly.

The SpERC is not intended to provide a definitive estimate of environmental exposure at the local scale. It must be combined with use of the LET.

The CLE SpERC, when selected in ECETOC TRA or Chesar, is used to estimate the contribution to the regional background concentrations ($PEC_{regional}$) from the use of treated seeds/granular PPP; any local scale PECs calculated in ECETOC TRA or Chesar should be disregarded. The emission factors encoded in the SpERC can also be transferred to other tools to calculate the regional background PECs, e.g. EUSES.

Following import of the $PEC_{regional}$ into the LET, the treated seed/granular scenario can be run to estimate local PECs.

PC 27: Delivery and dispersion of agrochemical plant protection products

Description of the activities and technical processes: Manual spreading by hand/spoon/cup, push rotary spreader, or belly grinder, of granular plant protection products or treated seeds on residential lawns/turf, gardens (flowers, fruits, vegetables), and trees (fruits, nuts, shrubs, ornamentals).

The worst-case "sentinel" value for these sub-activities is carried forward as the generic conservative exposure value for manual spreading activities in the contributing scenario for risk assessment.

1.3.5 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 model 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.

1.3.6 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 4.1) 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

A specific tool (CLE OWB) 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 covers professional workers and consumers exposed 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 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 e.g. to ECETOC TRA which lacks 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.

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)

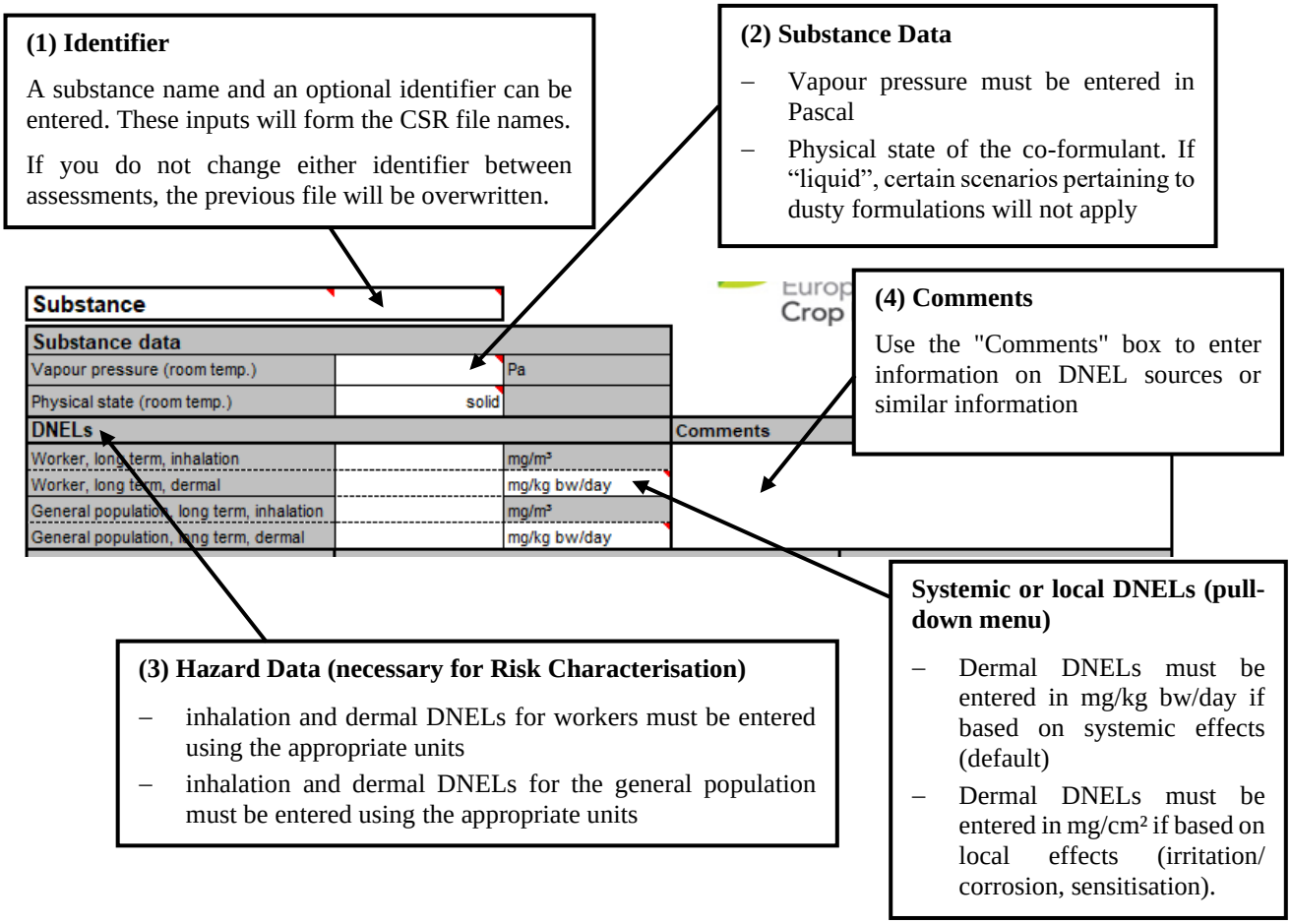
  - Generates outputs in .docx format
  - Hand surface of consumers is 840 cm² instead of 960 cm² for workers, in alignment with REACH GD R.15
  - CSR Format now based on the ECHA template implemented in IUCLID 5.6
  - Macro buttons now implemented as Form Buttons, not ActiveX controls for better version-to-version stability
- V3.3 (October 2015)
  - Fixed a situation that allowed bystander RCRs to exceed 1 after using the maximisation function
- V4.0 (October 2016, and later bug fixes)
  - The underlying exposure models were changed from the German model to the 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
  - Seed treatment has been removed from the OWB tool, because of the currently ongoing development of a designated model for the estimation of operator exposure during seed treatment
  - An error in the RCR calculation formula for PPR GES2 has been fixed (February 2019).
  - An error in the calculation of vapour drift exposure has been fixed (July 2019).
  - RCRs are calculated for all routes/populations for which a DNEL is entered (July 2019).
  - 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 (July 2019).
  - Exposure to spray and vapour drift is now considered relevant for workers only (October 2020).
  - TCs for crop-type "General" are used as default for re-entry workers (October 2020).
  - Residential exposure via drift and surface deposits is not considered relevant for substances with low toxicity (October 2020).
  - Upwards or downwards hand-held spraying are carried forward to risk assessment, depending on which gives the worst-case combined RCR (October 2020).

2.4 User guidance

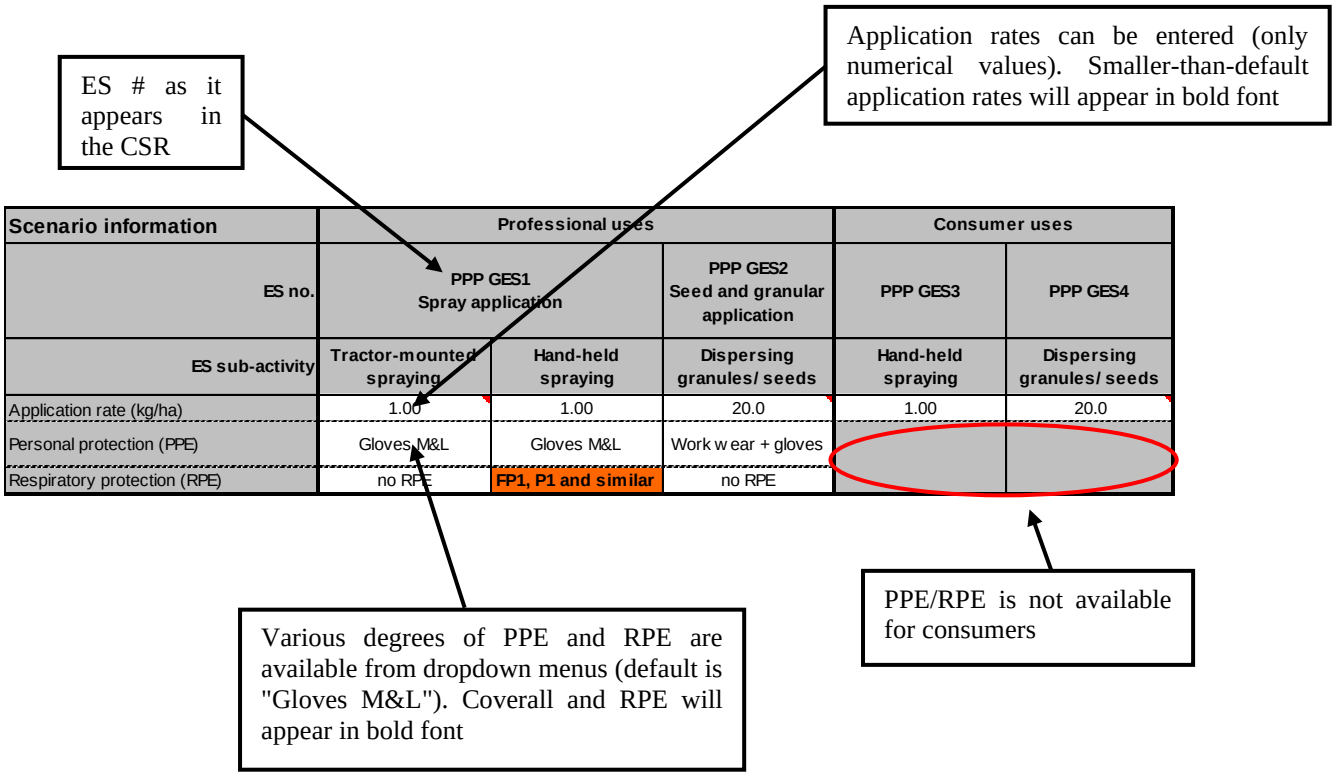
2.4.1 Inputs

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

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



2.4.2 Scenario information



Scenario information	Professional uses			Consumer uses	
ES no.	PPP GES1 Spray application		PPP GES2 Seed and granular application	PPP GES3	PPP GES4
ES sub-activity	Tractor-mounted spraying	Hand-held spraying	Dispersing granules/ seeds	Hand-held spraying	Dispersing granules/ seeds
Application rate (kg/ha)	1.00	1.00	20.0	1.00	20.0
Personal protection (PPE)	Gloves M&L	Gloves M&L	Work wear + gloves		
Respiratory protection (RPE)	no RPE	**FP1, P1 and similar**	no RPE		

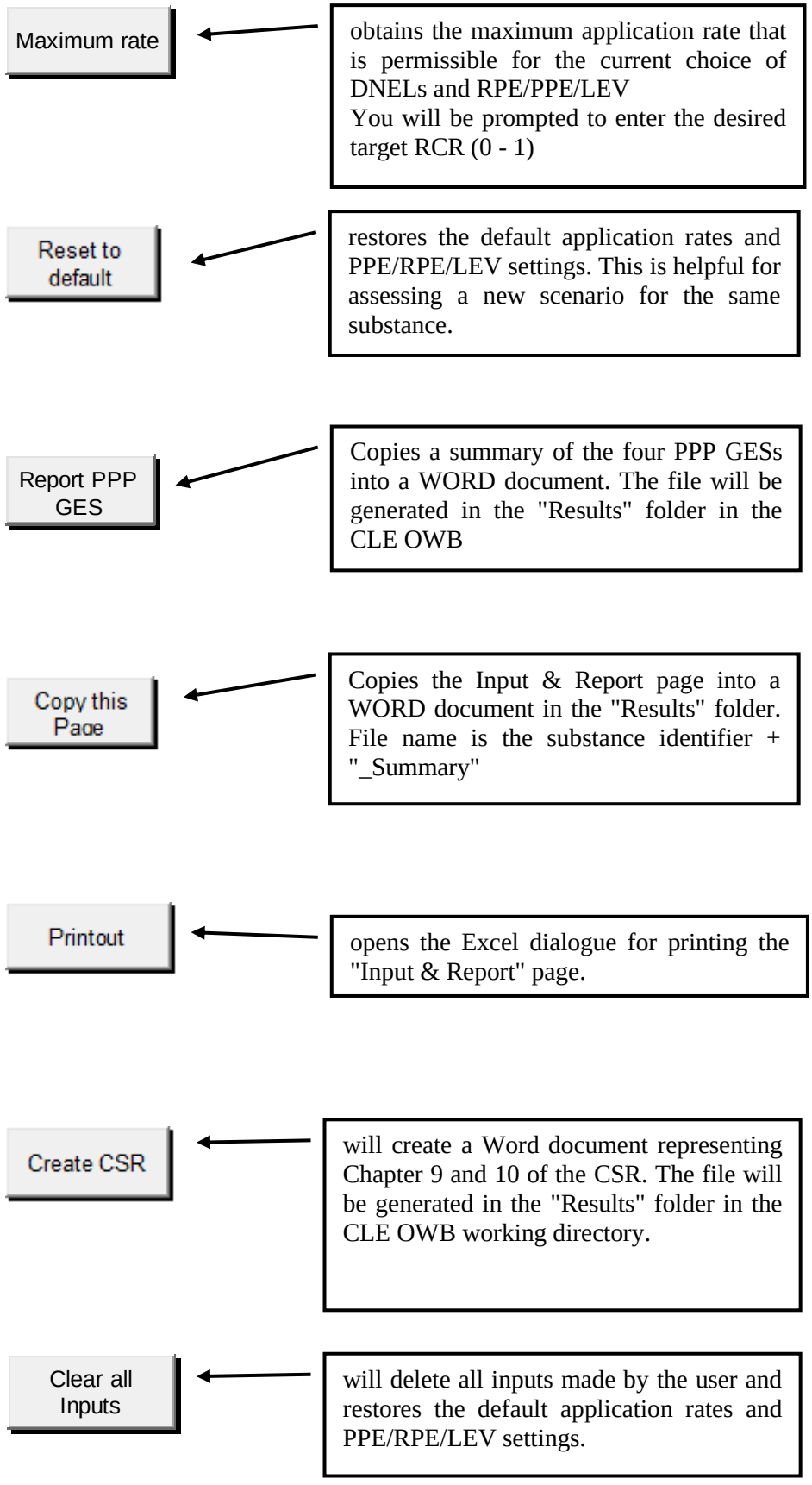
2.4.3 Results

The “Results” table will be populated as the necessary hazard and scenario information are entered. The table summarizes all input parameters and the resulting exposure estimates.

Results		
Inhalation exposure [mg/m³]		
Mixing / loading (PROC 8a)	0.056	0.0050
Application (PROC 8b, 11 or 8a)	0.014	0.350
RCR inhal	0.070	0.355
Dermal exposure [mg/kg bw/day]		
Mixing / loading (PROC 8a)	0.0069	2.93
Application (PROC 8b, 11 or 8a)	1.31	0.577
RCR dermal	0.661	1.75
Combined routes		
RCR total	0.731	2.11

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 cut-and-pasting the respective output tables generated by LET.

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.

The **conclusion on risk characterisation** has to be added at the **end of each contributing scenario.** The conclusion has to 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 worst-case reasonable 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/m³]	PPE	RPE	Dermal RCR	Inhalation RCR	Total RCR
	[kg/ha]	[kg/d]							
Tractor-mounted boom spraying									
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
PROC 8a+11			**0.993**	**0.696**			**0.993**	**0.696**	**1.689**
Tractor-mounted air-blast spraying									
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
PROC 8a+11			**0.762**	**0.454**			**0.762**	**0.454**	**1.216**
Hand-held spraying									
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
PROC 8a+11			**0.571**	**0.003**			**0.571**	**0.003**	**0.574**

2.5 Model Information summary

2.5.1 Introduction

Assessment of agrochemical uses

CropLife Europe (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 human exposures is presented as a table within the contributing scenario. However, only the worst-case exposure is selected and carried forward for risk characterisation.

In accordance with ECHA Guidance Chapter R.14: Occupational exposure estimation and ECHA Guidance Chapter R.15: Consumer exposure estimation, the following general parameters for exposure assessment are used (ECHA R.14, 2016 and ECHA R.15, 2016):

- Body weight, adults: 60 kg
- Respiratory volume, worker: 10 m^3/ 8 h
- Respiratory volume, general population: 20 m^3/ 24 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 output 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; and 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 of bystanders.

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

A number of established models are available for the assessment of operator exposure to (active) substances in PPP. The European Food Safety Agency (EFSA) reviewed available studies on operator exposure to PPP and developed the "Agricultural operator exposure model" (AOEM) to be used in the risk assessment of PPP in Europe (EFSA, 2014). The AOEM is mainly based on a joint project for the development of an agricultural operator exposure model (Groβkopf *et al.*, 2013) to replace older exposure models, such as the "German BBA model" (Lundehn *et al.*, 1992).

The AOEM is based on more than 30 exposure studies generated between 1994 and 2009, predominantly in the context of plant protection product authorisation in Europe. Studies were included after evaluation according to a set of quality criteria. A statistical analysis of the exposure data resulted

in six validated models for the use of PPP. Of these, five models are predicting exposure as a function of the amount of substance used per day and other contributing parameters. In the case of mixing and loading of knapsack and downward spraying with hand-held equipment, the number of data points was too small to show a clear correlation of the magnitude of the measured exposure and the amount of substance used. The percentiles of the exposure distribution were calculated and used directly in this case. These percentiles of the exposure distribution cover the application of up to 1.5 kg of substance per day; exposure values for larger amounts can be obtained by linear extrapolation. The derived exposure models for the prediction of operator exposure cover the mixing and loading and outdoor application of PPP by downward and upward spraying with vehicle-mounted, vehicle-trailed and hand-held equipment including active substances with vapour pressures of up to 0.01 Pa.

Further models were included in the AOEM, to predict operator exposure resulting from the handling of granular products (e.g., the US Environmental Protection Agency Pesticide Handler Exposure Database, PHED).

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 AOEM can be translated into the REACH process category PROC 8a.

Unless specified, the AOEM assumes no protective clothes are worn, i.e. workers wear normal work clothing consisting of T-shirt, trousers, and shoes.

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 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 which therefore usually constitutes the worst case, unless gloves are worn during mixing and loading. In this case, air-blast spraying may become the worst-case for tractor-mounted applications.

For 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. The corresponding amount of substance handled per day is considered for assessing exposure 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 amount of exposure (µg substance per day) is assumed for both M&L and application. 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 vs. 1 ha/day for knapsack sprayers) is therefore used as worst-case scenario covering all types of hand-held applications. Both upward and downward spraying directions are considered for hand-held spraying 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 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 AOEM.

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 AOEM 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/m³]	Total RCR
Mixing and loading tractor mounted/trailed boom sprayer	AOEM	Liquid	0.023	0.0009	0.024
		Powder (WP)	0.352	0.5053	**0.857**
		Granule (WG)	0.007	0.0087	0.016
Mixing and loading tractor mounted/trailed broadcast air-assisted sprayer	AOEM	Liquid	0.005	0.0005	0.006
		Powder (WP)	0.094	0.3130	0.407
		Granule (WG)	0.002	0.0054	0.007
Mixing and loading hand-held sprayer, outdoors or indoors	AOEM	Liquid	0.009	0.0006	0.010
		Powder (WP)	0.153	0.0108	0.164
		Granule (WG)	0.003	0.0108	0.014

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

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 AOEM 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 AOEM assumes that no protective clothes are worn, i.e. workers wear normal work clothing consisting of long-sleeved shirt, trousers, socks, and shoes.

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. AOEM 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 spraying with lances connected to a large tank or a knapsack tank, respectively.

Table 2: Typical CLE OWB output table (PROC11) showing exposure estimates for all variable exposure determinants: four possible tasks within the AOEM 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]	Oral exposure [mg/kg bw/day]	Inhalation Exposure [mg/m³]
Tractor mounted/trailed boom spraying	AOEM*	Liquid	0.043		0.0004
Tractor mounted/trailed broadcast air-assisted spraying			0.198		0.0128
Hand-held spraying, downwards, outdoors			0.725		0.0108
Hand-held spraying, downwards, indoors (greenhouse)	CRRM*		0.725		0.0108
Worker re-entry (indirect exposure)	AOEM	Liquid	Negligible		Not assessed
Professional Bystander (indirect exposure)	AOEM	Liquid	0.7844		0.0169

*AOEM: Agricultural operator exposure model, CRRM: constant rate release model

The CRRM model used in addition to the AOEM in Table 2 is described in the following section.

2.5.2.4 Extending the exposure scenario to greenhouses

The highest exposure potential for co-formulants used in greenhouses is associated with application by hand-held spraying. Dermal and inhalation exposure to spray mist is assessed using the EFSA AOEM.

For volatile substances, vapours make a significant contribution to inhalation exposure in addition to spray mist. According to REACH Guidance Document R.7a (Section R.7.4.4.1), a substance is non-volatile in the context of indoor scenarios, if its vapour pressure is below 0.01 Pa (ECHA R.7a, 2017).

This additional component of inhalation exposure is simulated using the constant rate release model (CRRM) described in the following section. A cut-off for volatility was set at 0.1 Pa in accordance with the CRRM, which assumes that the applied volatile substance is instantaneously vaporised and distributed to the available airspace.

Constant Rate Release Model (CRRM)

The ConsExpo methodology is used to assess the additional contribution of vapour inhalation. The constant rate release model used in ConsExpo (RIVM, 2005) was considered to be a useful approach, particularly because of the limited number of input parameters required. This model deals with a known quantity of substance released continuously over a defined period, within a defined space (volume). It is assumed that the substance is immediately volatilised on release, allowing the concentration to build, while simultaneously being removed by natural ventilation. The following equation for calculating the concentration in air at a given time was provided (see reference, Equation 3a):

$$C_{air} = \frac{A_0 \cdot Wf}{q \cdot V \cdot tr} \cdot \left(1 - e^{-qt}\right)$$ **Equation 1**

The equation given was integrated for use in the OWB model as follows:

$$\int_0^t C_{air}(t) \cdot dt = \int_0^t \frac{A_0 \cdot Wf}{q \cdot V \cdot tr} \cdot \left(1 - e^{-qt}\right) \cdot dt$$ **Equation 2**

$$= \left[\frac{A_0 \cdot Wf}{q \cdot V \cdot tr} \cdot t + \frac{A_0 \cdot Wf}{q^2 \cdot V \cdot tr} \cdot e^{-qt} \right]_0^t$$ **Equation 3**

$$= \frac{A_0 \cdot Wf}{q \cdot V \cdot tr} \cdot t + \frac{A_0 \cdot Wf}{q^2 \cdot V \cdot tr} \cdot e^{-qt} - \frac{A_0 \cdot Wf}{q^2 \cdot V \cdot tr}$$ **Equation 4**

where:

C_{air} = concentration of the substance in the greenhouse air	[kg.m^{-2}]
A_0 = mass of the substance applied	[kg]
Wf = weight fraction of the substance in the formulation applied	[fraction]
q = number of air changes per unit time	[h^{-1}]
V = volume of air in the greenhouse	[m^3]
tr = duration of substance release to air	[h]
t = total exposure time	[h]

C_{air} = 0 mg m^{-3} at t = 0 h, and t = t_r for this case where exposure and substance release period are correlated and correspond only to spraying activity within the greenhouse.

The Equation 4 can be further simplified and adapted for the greenhouse assessment scenario. Substances are considered only in terms of their application rate, and as such the weight fraction term is redundant i.e. Wf = 1. Furthermore, the application rate is the typical descriptor available, rather than the total mass. As such the following relations can be derived: *Mass = Rate x Area* and *Volume = Area x Height* and Equation 4 simplified to:

$$\frac{AR}{q \cdot h \cdot tr} \cdot t + \frac{AR}{q^2 \cdot h \cdot tr} \cdot e^{-qt} - \frac{AR}{q^2 \cdot h \cdot tr}$$ **Equation 5**

where:

AR = application rate of the substance	[kg.ha^{-1}]
h = height of the greenhouse	[m]

The T hour time weighted average (TWA) is given generically by:

$$T \text{ hour TWA} = \frac{1}{T} \int_0^t C_{air}(t) \cdot dt$$ **Equation 6**

where:

T = period over which the exposure is averaged	[h]

and

$$T \text{ hour TWA} = \frac{1}{T} \cdot \left(\frac{R}{q \cdot h \cdot tr} \cdot t + \frac{R}{q^2 \cdot h \cdot tr} \cdot e^{-qt} - \frac{R}{q^2 \cdot h \cdot tr} \right) \cdot 100$$ **Equation 7**

where:

T hour TWA = time weighted average, e.g., 8-h TWA [mg.m^{-3}]

100 = conversion factor kg.ha^{-1} to mg.m^{-2}

From Equation 7 it is apparent that the worker exposure to a volatile substance will depend only on the application rate, ventilation rate, height of the greenhouse, and exposure duration. As described previously, the exposure is independent of vapour pressure because it is assumed for substances with a vapour pressure ≥0.1 Pa that evaporation is immediate.

The following default values and assumptions were used.

Variable	Value	Comment
tr = t	6 h	Assumes emission only occurs during spraying. Duration is the standard assumption in crop protection exposure assessments and represents a worst-case of 6 hour spraying within a single contiguous greenhouse.
t	8 h	Assumes no exposure for remaining duration of the working period, and a standard 8 hour working day for DNEL comparison.
h	3 m	Height is the standard assumed in crop protection greenhouse assessments. The concentration of the volatile substance increases with a lower greenhouse height, due to the smaller volume of air available for dilution of the unit application rate.
AR	1 kg.ha^{-1} (or maximised)	Default application rate (or maximised to a specified RCR).
q	1 h^{-1}	Natural “good” ventilation. Mechanically ventilated greenhouses would have a higher exchange rate.

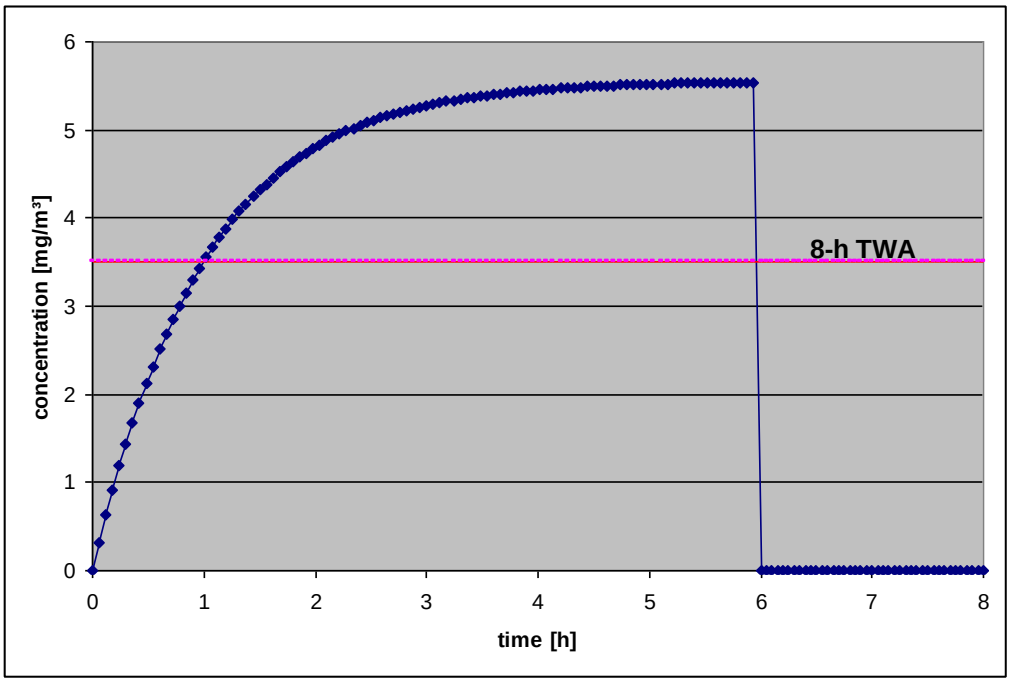
The worst case for volatiles becoming airborne is instantaneous evaporation immediately after release by spraying. The overlay of this continuous release vs. removal by ventilation has been simulated using the ConsExpo model (see Figure 1). Exposure ceases after 6 hours when the operator is expected to leave the greenhouse.

Using Equation 7 and the default parameters listed in the table above, the 8-h TWA is:

$$\text{TWA}_{8h} = AR \cdot 3.47 \text{ mg/m}^3$$ **Equation 8**

With *AR* being the application rate of the co-formulant [kg/ha]

Figure 1: Simulation of vapour concentration (continuous release of $A_0 = 1$ kg over a period of $t = t_r =$ 6h, with ventilation $q = 1\ h^{-1}$, in a space with volume $V = 30\ 000\ m^3$). The period from 6-8 h corresponds to when the worker has left the greenhouse.



Where the vapour pressure of a substance is ≥0.1 Pa, its immediate and complete evaporation as it is released from the spray nozzle is assumed. For such substances, exposure to vapour is calculated using Equation 8. These cases are indicated in output tables as "CRRM", the constant rate release model. For substances with lower vapour pressures, only spray exposure (from the AOEM model) is considered relevant.

2.5.2.5 Consideration of Worker Re-entry

While not explicitly considered in industrial exposure assessments, worker exposure resulting from re-entry is included here as it forms part of the typical risk assessment paradigm used in agrochemical exposure assessments. Because exposure arising from worker re-entry is not a formal 'use' of the substance, the use descriptor system is not applicable in this case.

Workers re-entering treated cultures are potentially exposed to dislodgeable foliar residues (DFR). If a co-formulant is volatile (at this time scale defined as vapour pressure ≥0.1 Pa), then the DFR is zero 24 hours after application due to complete evaporation of the substance.

The only significant potential for worker exposure following re-entry will be contamination via the skin. Inhalation exposure is considered to be negligible. For non-volatile co-formulants, the default initial DFR of 3 µg/cm² per kg substance/ha is adopted from AOEM. External dermal exposure of workers (re-)entering treated cultures ($E_{D,\ worker}$) is calculated within AOEM using the following equation:

$$E_{D,\ worker}\ [mg/kg\ bw/day] = TC \times ET \times DFR_{initial} \times AR / 1000 / BW \qquad \textbf{Equation 9}$$

Where:

TC: transfer coefficient [cm²/h]

ET: exposure time [h/day]

$DFR_{initial}$*:* dislodgeable foliar residue [µg/(cm² × kg/ha)]

AR: application rate [kg/ha]

BW: body weight [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 approach.

Considerations on Transfer Coefficients:

AOEM has transfer coefficients (TCs) for twenty different crop types with matching exposure times. These options have been made available in OWB as well. However, registrants 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 75th percentile TC for the "general crop" category given in the EFSA AOEM guidance (EFSA, 2014). 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 cm²/h). TCs for gloved hands are not available for the general crop category. As a surrogate, the respective TC of 580 cm²/h is adopted from vegetables (Table 3).

Where a local risk assessment is required, dermal exposure is normalised to the palmar surface of both hands, with an assumed surface area of 420 cm². 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.

In this default scenario, inhalation of vapours of the co-formulant is not relevant, in accordance with the assumptions made in the AOEM.

Table 3: Exposure Parameters for Workers

Variable	Value	Unit	Explanation
TC	1400	cm²/h	Transfer coefficient, normal work clothing, 75th percentile
	580		Transfer coefficient, normal work clothing plus gloves, 75th percentile
ET	8	h/day	Daily exposure duration
$DFR_{initial}$	3	µg/(cm² × kg/ha)	Dislodgeable foliar residue, normalised to application rate
BW	60	kg	Body weight, adults

2.5.2.6 Consideration of Exposure of Bystanders

While not explicitly considered in 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 in agrochemical exposure assessments. Exposure of bystanders occurs as a result of the use of the substance, but it is not a "use" itself. The use descriptor system is therefore not applicable in this case.

Dermal exposure to spray drift can occur for individuals that are present in the vicinity of cultures undergoing spray treatment. For occasional bystanders and residents, this entails acute exposure. Short-term DNELs for the general population have only been set for few substances used as co-formulants in PPP. In the absence of short-term DNELs, the use of long-term DNELs for assessing acute exposure to co-formulants without appreciable acute toxicity is not considered relevant or useful. Even though OWB offers the option of conducting risk assessments for such toxic substances, it is recommended that a refined expert assessment be conducted on a case-by-case basis. Such uses are not within the scope of a screening-level assessment. The use of highly toxic substances as co-formulants in PPP is discouraged. Furthermore, PPP GES 3 and 4 describe amateur use of PPP as spray, granular or seed application and can be used to assess direct consumer exposure to co-formulants used in PPP, if consumer exposure is considered to be relevant.

Repeated, regular exposure to spray drift can be relevant for agricultural workers working in the vicinity of an ongoing spray application. In the following, the term "bystander" refers to workers carrying out activities in the area of PPP application but who are not operators. Bystanders can be exposed to spray and /or vapour drift from such applications.

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

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

$$E_{D,\,drift}\ (mg/kg\ bw/day) = DE_{drift} \times (1\text{-}LCAF) \times C_{dil} \times 1000 / BW \qquad \textbf{Equation 10}$$

Where:

DE_{drift} = dermal exposure to spray drift (mL/person)

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

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

BW = body weight (kg)

Drift data are adopted from the EFSA AOEM (EFSA 2015). A distance of 10 m from the spray equipment aiming in upward direction 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 Bystanders

Variable	Value	Unit	Explanation
DE_{drift}	1.689	mL/person	dermal exposure of child to spray drift, upward spraying, 75th percentile
IE_{drift}	0.00170	mL/person	inhalation exposure of child to spray drift, upward, 75th percentile
LCAF	18%	%	Light clothing adjustment factor
BW	60	kg	Body weight, adult
IR	1.07	m³/day/kg bw	Inhalation rate, children
C_{vapour}	0.000	mg/m³	Concentration in air of substance with negligible volatility, i.e. VP* <0.00001 Pa
	0.001	mg/m³	Concentration in air of substance with low volatility, i.e. 0.00001 Pa < VP < 0.005 Pa
	0.015	mg/m³	Concentration in air of substance with medium or high volatility, i.e. VP ≥ 0.005 Pa

[a] VP: vapour pressure of the co-formulant at 25 °C

Inhalation exposure of bystanders to spray drift ($E_{I, drift}$) is based on the following equation:

$$E_{I, drift}\ (mg/m^3) = IE_{drift} \times C_{dil} \times 1000 / BW / IR \qquad \textbf{Equation 11}$$

Where:

IE_{drift} = inhalation exposure to spray drift (mL/person)

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

BW = body weight (kg)

IR = inhalation rate (m^3/day/kg bw)

2.5.2.7 Exposure estimation for combined contributing scenario worker exposure

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 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/m³]	PPE	RPE	Dermal RCR	Inhalation RCR	Total RCR
	[kg/ha]	[kg/d]							
Tractor-mounted boom spraying									
PROC 8a: Mixing & loading WP formulation	**0.34**	**17.09**	0.352	0.5053	gloves	no RPE	0.352	0.5053	0.857
PROC 11: Tractor-mounted boom spraying			0.043	0.0004	no PPE	no RPE	0.043	0.0004	0.043
PROC 8a+11			**0.394**	**0.506**			**0.394**	**0.506**	**0.900**
Tractor-mounted air-blast spraying									
PROC 8a: Mixing & loading WP formulation	**0.34**	**3.42**	0.094	0.3130	gloves	no RPE	0.094	0.3130	0.407
PROC 11: Tractor-mounted air-blast spraying			0.198	0.0128	no PPE	no RPE	0.198	0.0128	0.210
PROC 8a+11			**0.291**	**0.326**			**0.291**	**0.326**	**0.617**
Hand-held spraying									
PROC 8a: Mixing & loading WP formulation into hand-held sprayer	**1.56**	**6.24**	0.153	0.0108	gloves	no RPE	0.153	0.0108	0.164
PROC 11: Hand-held spraying, indoors (greenhouse)			0.725	0.0108	no PPE	no RPE	0.725	0.0108	0.736
PROC 8a+11			**0.878**	**0.022**			**0.878**	**0.022**	**0.899**

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 as granular applications or 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, and the loading of manual belly-grinders and "push-type" spreaders; the transfer of treated seeds from a batch treater into bags; and 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 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 AOEM implementation of US Environmental Protection Agency "The Pesticide Handler Exposure Database" (PHED, scenario Mixing/Loading Granules)[1] and the following equations:

$$E_{dermal} = \frac{AR \cdot A \cdot UE_{route}}{BW} \quad \text{[mg/kg bw/day]} \qquad \textbf{Equation 12}$$

$$E_{inh} = \frac{AR \cdot A \cdot UE_{route}}{RV} \quad \text{[mg/m³]} \qquad \textbf{Equation 13}$$

Where:

E_{dermal} = Dermal exposure, systemic	[mg.kg.bw^{-1}]
E_{inh} = Inhalation exposure	[mg.m^{-3}]
AR = Application rate	[kg.ha^{-1}]
A = Area	[ha.day^{-1}]
UE_{route} = Unit exposure for the relevant route and quantity handled	[mg.kg^{-1}]
BW = Body weight	[kg]
RV = Respiratory volume	[m³.day^{-1}]

The following default values and assumptions were used for loading granular PPP or treated seeds:

Variable	Value	Comment
AR	20 kg.ha^{-1} (or maximised)	Default application rate (or maximised to a specified RCR)
A	50 ha	Default area for tractor
UE_{body}	0.0162 mg.kg^{-1}	Unit value per kg substance handled, light clothing
UE_{hand}	0.002 mg.kg^{-1}	Unit value per kg substance handled, gloves
$UE_{inhalation}$	0.0208 mg.kg^{-1}	Unit value per kg substance handled, no RPE
BW	60 kg	AOEM default
RV	10 m³.day^{-1}	REACH worker default, light work

[1] 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)

Exposure values are 75th 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). 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 6: 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^3]	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]

A separate tool for the assessment of seed treatment is currently being developed outside of the REACH-IN project. The OWB tool currently does not contain models that can be used to assess seed treatment, but an extension will be considered when the dedicated models for seed treatment are becoming public.

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

Dispersion of granular PPP or pre-treated seeds can be conducted manually (spreading by hand) or using either hand-held or tractor-mounted equipment. The PHED model is used to assess exposure resulting from handling granular materials. In its implementation by the AOEM, only dispersion by hand or tractor-mounted equipment is covered. The activity can be translated into the systematic use descriptor PROC 8a. Manual dispersion by hand is assumed to apply to smaller areas not exceeding 200 m² according to PHED, but the area in the AOEM was increased to 1 ha per day.

Exposure from this application type is assessed using The Pesticide Handler Exposure Database (PHED; US EPA, 2012). Use of working clothes (long-sleeve shirt, long pants, shoes plus socks) is assumed in the PHED exposure predictions. 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 PPPs by multiplying actual exposure values with an assumed protection factor of 100. This approach is adopted in OWB.

The default work rate using tractor-mounted equipment is 50 ha per day and the use rate for manual dispersion is 1 ha per day.

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 low compared to the dermal route. The exposure during application of granular PPP or pre-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 12 and Equation 13) for calculation of exposures from PHED. The following default values were used in addition to those previously specified:

Scenario	Variable	Value	Comment
Applicator, Granules by Hand	UE_{body}	68.87 mg/kg substance	Unit value for covered body per kg handled, no PPE
	UE_{hand}	14.27 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_{dermal}	0.004694 mg/kg substance	Unit value for covered body per kg handled, no PPE
	UE_{hand}	0.00408 mg/kg substance	Unit value for hand per kg handled, gloves
	$UE_{inhalation}$	0.00119 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 $kg.ha^{-1}$ (or maximised)	Default application rate (or maximized to a specified RCR)

Table 7: 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^3]	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 8: 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/m³]	Dermal RCR	Inhalation RCR	Total RCR
	[kg/ha]	[kg/d]					
Dispersion of granules or treated seeds, tractor							
PROC 8a: Mixing and loading granules (including treated seeds)	**0.628**	**31.4**	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
PROC 8a+8a			**0.011**	**0.074**	**0.011**	**0.074**	**0.085**
Dispersion of granules or treated seeds, manual							
PROC 8a: Spreading of granules or treated seeds by hand	**0.628**	**0.628**	**0.871**	**0.029**	**0.871**	**0.029**	**0.900**

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; and 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^2/day) than professional use (1 to 50 ha/day). It cannot be anticipated that consumers wear PPE during the application of PPP. The AOEM 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 (ca 1 kg/ha) for co-formulants. However, the AOEM algorithms do not allow scaling down to smaller, more realistic application rates. Therefore, the German BBA model (Lundehn *et al.*, 1992) is used for hand-held applications, because it allows linear scaling of exposure estimates in relation to any application rate.

The consumer use of PPP predominantly results in dermal and inhalation exposure. 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 PPs is considered to be accidental and beyond a reasonable worst-case scenario.

The 75th percentile exposure parameters from the "German BBA Model" database are used in OWB calculations (Table 9). The amateur use implies that no protective clothes or gloves are worn. Consumers are assumed to wear light clothes consisting of T-shirt, shorts and shoes.

Table 9: 75th percentile indicative exposure parameters from the BBA model

	Liquid	WG	WP
M&L			
Hand contamination mg/kg a.s.	430.25	171.4	171.4
Inhalation exposure mg/kg a.s.	0.0967	0.0628	1.534
Spraying			
Dermal contamination mg/kg a.s.			
Head	17.445		
Hand	29.125		
Rest of body	142.55		
Inhalation exposure mg/kg a.s.	0.824		

The contributing scenario covers the mixing and loading of the preparation into a hand-held sprayer. PPP can be a liquid, granular or powder formulation. While the BBA model does not contain dermal exposure data for mixing and loading of powder formulations (WP), the respective data for liquid formulations are chosen as surrogate.

The contributing scenario also covers the dispersion of the diluted PPP using a hand-held sprayer. Spraying to high targets (e.g. trees) has a higher potential for exposure than spraying to low targets (e.g. potatoes), and therefore is conservative and considered to cover the latter case.

The outdoor use of PPP by amateurs covers spraying to high targets and a treatment area up to 200 m^2. Indoor uses by amateurs will cover much smaller treatment areas. Therefore, the outdoor scenario provides a worst-case exposure estimate for amateur indoor uses. No separate model calculation is presented for the indoor spraying by amateurs.

Table 10: 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/m³]	Total RCR
Mixing and loading hand-held sprayer, outdoors	BBA	Liquid	0.620	0.00061	0.6204
		Granule (WG)	0.247	0.00039	0.2473
		Powder (WP)	0.247	0.00961	0.2565
Hand-held spraying, high-level target, outdoors		Liquid	0.272	0.0071	0.2796

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 11. The combined exposure is carried forward for risk assessment.

Table 11: 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/m³]	Dermal RCR	Inhalation RCR	Total RCR
	[kg/ha]	[g/d]					
Task 1: Mixing & loading liquid formulation into knapsack sprayer	**4.32**	**86**	0.620	0.0006	0.620	0.0006	0.6204
Task 2: Hand-held spraying, outdoors			0.272	0.0071	0.272	0.0071	0.280
Task 1 + 2			**0.892**	**0.008**	**0.892**	**0.0077**	**0.900**

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 applications 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 pre-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)[2] using Equation 14 and Equation 15, assuming 100% absorption, as modified below:

[2] 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 (accessed 8 Jun 2012))

$$E_{dermal} = \frac{AR \cdot A \cdot UE_{route}}{BW \cdot Cf}$$ **Equation 14**

$$E_{inh} = \frac{AR \cdot A \cdot UE_{route}}{RV \cdot Cf}$$ **Equation 15**

Where:

E_{dermal} = Dermal exposure, systemic	[mg.kg.bw^{-1}]
E_{inh} = Inhalation exposure	[mg.m^{-3}]
AR = Application rate	[kg.ha^{-1}]
A = Area	[ha]
UE_{route} = Unit exposure for the relevant route and quantity handled	[µg.lb^{-1}]
BW = Body weight	[kg]
RV = Respiratory volume	[m³]
C_f = lb to kg conversion factor	[kg.lb^{-1}]

The daily work rate for 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 12: 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/m³]	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	**0.900**

*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

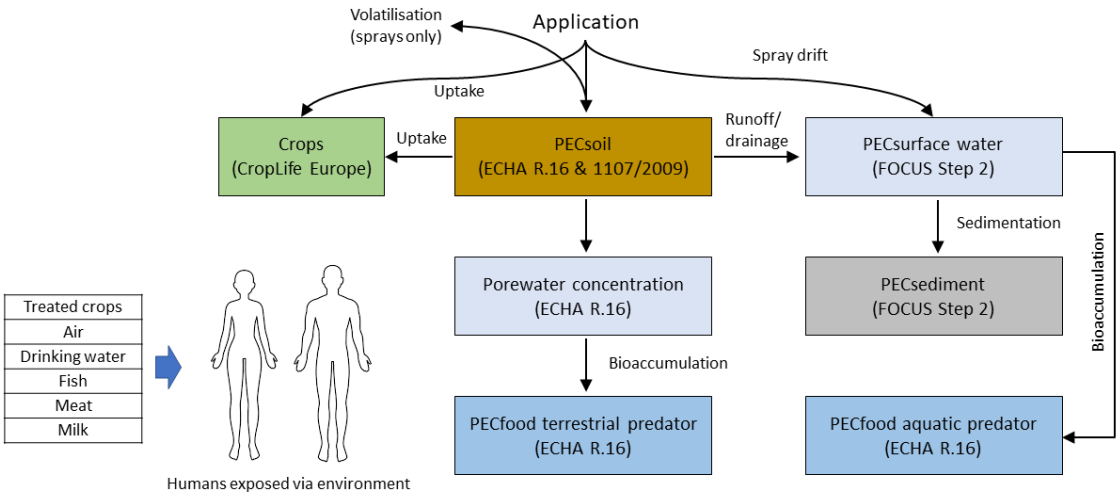
3.1 Introduction

Predicted Environmental Concentrations (PEC values), for various environmental compartments, and risk characterisations (via Risk Characterisation Ratios; RCR values), for various environmental receptors (such as aquatic organisms and terrestrial organisms), are required to be calculated as part of the REACH Environmental Risk Assessment for co-formulants. This is then presented in the relevant chapters on environmental exposure and risk assessment in the Chemical Safety Report (CSR), alongside the human health risk assessment.

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 PECs, associated with the use of the substance as a co-formulant in plant protection products and its other uses in other life cycle stages. The second step is to conduct a local scale assessment for use just as a co-formulant. The local scale assessment generates local concentrations for each relevant compartment that are then combined with the regional PECs to generate local PECs that are used in the risk characterisation.

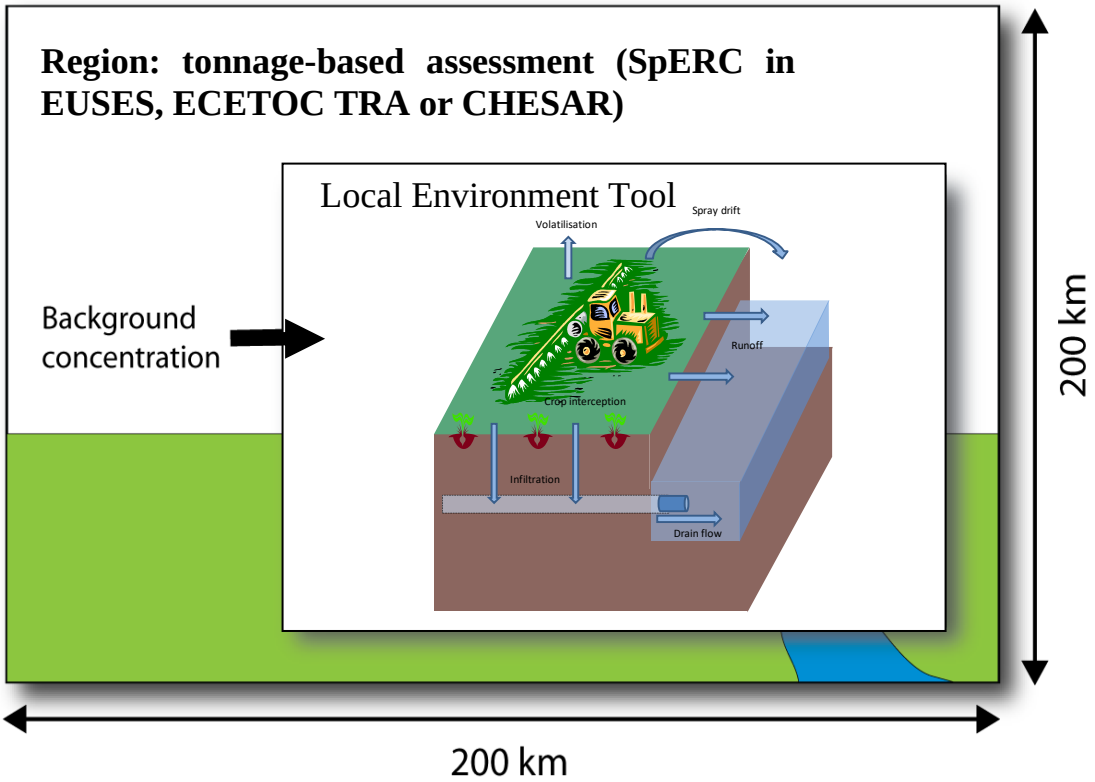
Regional scale estimates should be calculated outside the LET with appropriate tools using the defined emission factors of the CLE SpERCs (e.g. ECETOC TRA, EUSES, Chesar etc), and can be imported into LET.

The CLE Local Environment Tool (LET) calculates local-scale exposure estimates and combines with regional estimates to perform risk characterisations which conform to the requirements of REACH. The LET is a simple spreadsheet which facilitates quantitative local-scale assessments for all REACH relevant environmental compartments (including soil and surface water and secondary poisoning via the food chain). 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 (also referred to as the EU Technical Guidance Document on Risk Assessment (EU-TGD, 2003) calculations, as they were originally derived from the EU-TGD), 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:



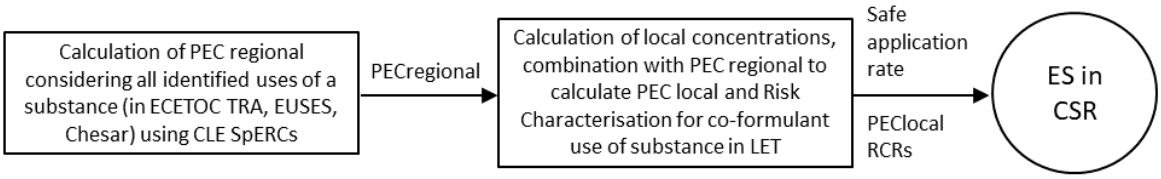
The calculations used in the LET for these assessments are discussed in detail in Section 3 (*Model information & user guidance*).

This scenario design is closely analogous to the established Tier 1 scenario used in the assessment of plant protection product active substances. 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 downstream users 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 downstream users manufacturing plant protection products.

On the other hand, upon receipt of the eSDS, downstream users 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 Downstream User 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. The easiest way to achieve this is by importing them 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_{50} 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.

If the user does not have an ECETOC TRA file with the required data, then manual entry 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 and to estimate the DT_{50} 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_{50} input to 'Manual input', after which the user can enter values in the appropriate boxes. DT_{50} 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_{OC}' on the QSAR dropdown list by default, and the user needs to manually enter an experimental K_{OC} 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_{OC} 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_{OC} value.

The LET will run without Regional PEC values being entered (zero values are assumed), but regional values 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[3], 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 (*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] 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.

3.4 'Refinement Options' of the LET

By 'Default', the tool is run for a reasonable worst-case scenario. In this analysis assumptions are made about the region and crop the substance is applied to and the timing of application. 'Assessment Type: Default' assumes a single application of the substance. At the end of a 'Default' analysis, an 'Estimated Safe Dose' is returned, and the RCR values for the environmental compartments are calculated using the Estimated Safe Dose (note: by default 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. 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 user the option to vary the scenario parameters to more closely represent their specific situation. This includes varying the usage 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 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 a 'Assessment Type: Refinement Options' assessment 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 (*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 (UVCB's), 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 ionizable substances

In particular, the LET can be used to screen for the risk associated with organic substances ionising at environmentally relevant pH values (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's they are neutral, whereas at other pH's 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).

Therefore, 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 [use $1x10^{-10}$ Pa in the LET], 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 $1x10^{-10}$ Pa and a K_{OW}/K_{OC} of zero. This is a worst case. The worst case RCR's for each compartment across the results from the two runs constitute the screening level assessment, and the worst-case 'Safe Dose' 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 pKa 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 user 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 A, Trapp S. (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 $PNEC_{secondary\ poisoning}$ 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 humans via environment assessment 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 user 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 13. 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 13: 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 14.

Table 14: 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	∞

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 15 and Table 16.

Table 15: 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_{50}, days)	Readily biodegradable, failing 10 day window (DT_{50}, days)	Inherently biodegradable (DT_{50}, days)	Not biodegradable (DT_{50}, 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_{OC} * fraction organic carbon in standard soil (0.02)

Table 16: 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_{50}, days)	Readily biodegradable, failing 10-day window (DT_{50}, days)	Inherently biodegradable (DT_{50}, days)	Not biodegradable (DT_{50}, 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_{OC} * fraction organic carbon in standard soil (0.02)

It should be noted that in the LET, the maximum DT_{50} 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_{50} values are reported at 20 °C as this is the standard temperature used by the underlying FOCUS calculations. Therefore, when manually entering DT_{50} 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_{50} 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_{50} 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_{50} from test temperature (20 °C) to environmental temperature (12 °C) is calculated according to Equation 16, in accordance with the EU-TGD (2003) and ECHA R.16 (2016) guidance.

$$DT_{50}soil_{12°C} = DT_{50}soil_{20°C} \times e^{(0.08 \times (20-12))}$$ **Equation 16**

Explanation of symbols

$DT_{50}soil_{20°C}$	Half-life of the co-formulant in soil at 20 °C	[d]	User input
$DT_{50}soil_{12°C}$	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 17 to Table 19.

Table 17: 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 18: Inferred Soil degradation rates at 20 °C reported in the LET on basis of biodegradability screening results and FOCUSsw guidance

Kpsoil (L.kg^{-1})	**Readily biodegradable (DT_{50}, days)**	**Readily biodegradable, failing 10-day window (DT_{50}, days)**	**Inherently biodegradable (DT_{50}, days)**	**Not biodegradable (DT_{50}, 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_{OC} * fraction organic carbon in standard soil (0.02)

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

Kpsoil (L.kg^{-1})	**Readily biodegradable (DT$_{50}$, days)**	**Readily biodegradable, failing 10-day window (DT$_{50}$, days)**	**Inherently biodegradable (DT$_{50}$, days)**	**Not biodegradable (DT$_{50}$, days)**
<100	158.2	474.6	1000	1000
>100, <1000	1000	1000	1000	1000
>1000, <10000	1000	1000	1000	1000

Kpsoil = K_{OC} * 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 17 to Equation 19.

$$Kp_{susp} = K_{OC} \times Foc_{susp}$$ **Equation 17**

$$K_{susp-water} = Fwater_{susp} + Fsolid_{susp} \times \frac{Kpsusp}{1000} \times RHOsolid$$ **Equation 18**

$$PNECsediment = \frac{K_{susp-water}}{RHO_{susp}} \times PNECsw \times 1000$$ **Equation 19**

Explanation of symbols

K_{OC}	Partition coefficient organic carbon -water	[L.kg^{-1}]	User input
Foc_{susp}	Fraction organic carbon in the suspended solids	[-]	0.1
$Fwater_{susp}$	Fraction water in suspended matter	[-]	0.9
Fsolid	Fraction solid in suspended matter	[-]	0.1
RHOsolid	Bulk density of solid phase	[kg.m^{-3}]	2500
PNECsw	Predicted no effect concentration in freshwater	[mg.L^{-1}]	User input
RHOsusp	Bulk density of wet suspended matter	[kg.m^{-3}]	1150
Kp_{susp}	Partition coefficient solid-water in suspended matter	[L.kg^{-1}]	
$K_{susp-water}$	Suspended matter-water partition coefficient	[m^3.m^{-3}]	
PNECsediment	Predicted no effect concentration in sediment (wet weight)	[mg.kg$_{wwt}^{-1}$]	

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 $PNEC_{marine\ water}$ is assumed to be $1/10^{th}$ 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.

$$PNECmarine\ water = \frac{PNECsurfacewater}{10}$$ **Equation 20**

Explanation of symbols

PNECsurface water	Predicted no effect concentration in freshwater	[µg.L^{-1}]	User input
PNECmarinewater	Predicted no effect concentration in marine water	[µg.L^{-1}]	

PNEC Marine water sediment derivation

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

$$PNECmarine\_sediment = \frac{K_{susp-water}}{RHO_{susp}} \times PNECmarinewater \times 1000$$ **Equation 21**

Explanation of symbols

$K_{susp\text{-}water}$	Suspended matter-water partition coefficient	[m^3.m^{-3}]	Equation 18
RHOsusp	Bulk density of wet suspended matter	[kg.m^{-3}]	1150
PNECmarinewater	Predicted no effect concentration in marine water	[mg.L^{-1}]	User input or Equation 20
PNECmarine sediment	Predicted no effect concentration in marine sediment (wet weight)	[mg.kg wwt^{-1}]	

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 $PNEC_{sediment}$ and $PNEC_{marine\ sediment}$ can be entered into the LET manually either in mg.kg$_{dwt}^{-1}$ or in mg.kg$_{wwt}^{-1}$. These units are converted using the following calculation:

$$PNECsed_{dwt} = PNECsed_{wwt} \times CONV_{susp}$$ **Equation 22**

$$CONV_{susp} = \frac{RHOsusp}{Fsolid_{susp} \times RHOsolid}$$ **Equation 23**

Explanation of symbols

$PNECsed_{wwt}$	Predicted No effect concentration in sediment (wet weight)	[mg.kg $_{wwt}^{-1}$]	User input
$CONV_{susp}$	Conversion factor for suspended matter concentration: wwt to dwt	[kg$_{wwt}$.kg$_{dwt}^{-1}$]	Equation 23

RHOsusp	Wet bulk density of suspended matter	[$kg_{wwt}.m^{-3}$]	1150
$Fsolid_{susp}$	Volume fraction of solids in suspended matter	[$m^3.m^{-3}$]	0.1
RHOsolid	Bulk density of solids	[$kg_{dwt}.m^{-3}$]	2500
$PNECsed_{dwt}$	Predicted No effect concentration in sediment (dry weight)	[$mg.kg_{dwt}^{-1}$]	

PNEC Soil derivation via equilibrium partitioning

The $PNEC_{soil}$ can also be estimated in the LET *via* the equilibrium partitioning method using Equation 24, in accordance with ECHA R.10 guidance (2008).

$$PNECsoil = \frac{K_{soil-water}}{RHOsoil} \times PNECsw \times 1000$$ **Equation 24**

Explanation of symbols

$PNEC_{sw}$	Predicted no effect concentration in freshwater	[$mg.L^{-1}$]	User input
RHOsoil	Bulk Density of wet soil	[$kg.m^{-3}$]	1700
Ksoil-water	Soil-water equilibrium partition coefficient	[$m^3.m^{-3}$]	Equation 42
$PNEC_{soil}$	Predicted no effect concentration in soil (wet weight)	[$mg.kg_{wwt}^{-1}$]	

Where the equilibrium partitioning method has been used to calculate the PNEC soil and the log Kow 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 $PNEC_{soil}$ can be entered into the LET manually either in $mg.kg_{dwt}^{-1}$ or in $mg.kg_{wwt}^{-1}$. These units are converted using the following calculation:

$$PNECsoil_{dwt} = PNECsoil_{wwt} \times CONV_{soil}$$ **Equation 25**

Explanation of symbols

$PNEC_{soil\ wwt}$	Predicted no effect concentration in soil (wet weight)	[$mg.kg_{wwt}^{-1}$]	User input
CONVsoil	Conversion factor for soil concentration wet-dry weight soil	[$kg_{wwt}.kg_{dwt}^{-1}$]	Equation 97
$PNEC_{soil\ dwt}$	Predicted no effect concentration in soil (dry weight)	[$mg.kg_{dwt}^{-1}$]	

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 25). 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 20.

Table 20: 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 26)

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 18 and it is assumed that these emission fractions apply for both indoor and outdoor use.

Table 21: 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
>0.000.1-0.001	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 26.

$$VP(TEMP_{standard}) = VP(TEMP_{test}) \times e^{\frac{H_{0vapour}}{R} \times \left(\frac{1}{273+TEMP_{test}} - \frac{1}{273+25}\right)} \quad \textbf{Equation 26}$$

Explanation of symbols

$VP(TEMP_{test})$	Vapour Pressure as give in the data set	[Pa]	User input
H_{0vapor}	Enthalpy of vaporisation	[J/mol]	5×10^4
R	Gas constant	[Pa.m^3.mol^{-1}.k^{-1}]	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 20). 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 22) (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 22: 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
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 23. 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 23: Crop interception values (FOCUS surface water Step 2)

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
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

Crop	No interception	F_{crop} (interception fraction)		
		Minimal crop cover	Intermediate crop cover	Full canopy
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
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.

$$Soil\ Loading = AR\ \times\ F_{soil} \times \left(1 - F_{crop}\right)$$ **Equation 27**

Explanation of symbols

AR	Application rate for co-formulant	[g.ha^{-1}]	User input
F_{crop}	Fraction of interception by crop (refinement option)	[-]	Table 23
F_{soil}	Emission factor to soil due to volatilisation of spray droplets (spray only)	[-]	Table 21
Soil Loading	Soil loading of the co-formulant	[g.ha^{-1}]	

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 20), 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:

$$Csoil_{initial} = \frac{Soil\ Loading \times\ 1000}{DEPTHsoil \times RHOsoil\ \times\ 10000}$$ **Equation 28**

Explanation of symbols

$DEPTH_{soil}$	Mixing depth of soil	[m]	Default: 0.05 Incorporation: 0.20
RHOsoil	Bulk density of wet soil	[$kg.m_{wwt}^{-3}$]	1700
Soil Loading	Soil loading of the co-formulant	[$g.ha^{-1}$]	Equation 27
10000	Area of 1 hectare	[m^2]	
$Csoil_{initial}$	Initial concentration in soil	[$mg.kg_{wwt}^{-1}$]	

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:

$$Csoil_{\max\_1} = Csoil_{initial}$$ **Equation 29**

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 30, losses due to volatilisation are calculated according to Equation 31 and losses due to leaching are calculated according to Equation 32. The equations describing loss processes are in accordance with ECHA guidance R.16.

$$kbio_{soil} = \frac{ln\,2}{DT_{50}bio_{soil}}$$ **Equation 30**

Explanation of symbols

$DT_{50}bio_{soil}$	Half-life for biodegradation in bulk soil at 12 °C	[d]	Equation 16
$kbio_{soil}$	first order rate constant for biodegradation in bulk soil	[d^{-1}]	

$$\frac{1}{k_{volat}} = \left(\left(\frac{1}{kasl_{air} \times K_{air-water}/K_{soil-water}} + \frac{1}{kasl_{soil}} \right) \times DEPTH_{soil} \right)$$ **Equation 31**

Explanation of symbols

$kasl_{air}$	Partial mass transfer coeff. at air side of the air-soil interface	[$m.d^{-1}$]	90.72
$kasl_{soil}$	Partial mass transfer coeff. at soil-side of the air-soil interface	[$m.d^{-1}$]	See ECHA R.16 guidance (2016), Equation R.16-59
$K_{air\text{-}water}$	Air-water equilibrium distribution constant	[$m^3.m^{-3}$]	Equation 44
$K_{soil\text{-}water}$	Soil-water partitioning coefficient	[$m^3.m^{-3}$]	Equation 42
$DEPTH_{soil}$	Mixing depth of soil	[m]	Default: 0.05 Incorporation: 0.20
k_{volat}	Pseudo first-order rate constant for volatilisation from soil	[d^{-1}]	

$$k_{leach} = \left(\frac{F\,inf_{soil} \times RAIN_{rate}}{K_{soil-water} \times DEPTH_{soil}}\right)$$ **Equation 32**

Explanation of symbols

$Finf_{soil}$	Fraction of rainwater that infiltrates into soil	[-]	0.25
RAINrate	Rate of wet precipitation (700 mm/year)	[$m.d^{-1}$]	1.92×10^{-3}
$K_{soil\text{-}water}$	Soil-water partitioning coefficient	[$m^3.m^{-3}$]	Equation 42
$DEPTH_{soil}$	Mixing depth of soil	[m]	Default: 0.05 Incorporation: 0.20
k_{leach}	Pseudo-first order rate constant for leaching from soil layer	[d^{-1}]	

The overall rate constant for these removal processes is given in Equation 33.

$$k = k_{volat} + k_{leach} + kbio_{soil}$$ **Equation 33**

Explanation of symbols

k_{volat}	Pseudo-first order rate constant for volatilisation from soil	[d^{-1}]	Equation 31
k_{leach}	Pseudo-first order rate constant for leaching from top soil	[d^{-1}]	Equation 32
$kbio_{soil}$	Pseudo-first order rate constant for biodegradation in soil	[d^{-1}]	Equation 30
k	First order rate constant for removal from top soil	[d^{-1}]	Equation 33

The maximum concentration in soil following multiple applications in one year is calculated with Equation 34.

$$Csoil_{\max\_1} = Csoil_{initial} \times \left(\frac{\left(1 - e^{(-k \times App\ Int)^{Napp}}\right)}{(1 - e^{(-k \times App\ Int)})}\right)$$ **Equation 34**

Explanation of symbols

$Csoil_{initial}$	Initial concentration in soil	[$mg.kg_{wwt}^{-1}$]	Equation 28
k	First order rate constant for removal from top soil	[d^{-1}]	Equation 33
App Int	Application interval	[d]	User input
Napp	Number of application events	[-]	User input
$Csoil_{max\_1}$	Maximum concentration in soil in year 1	[$mg.kg_{wwt}^{-1}$]	

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 35.

$$Facc = e^{-365 \times k}$$ **Equation 35**

Explanation of symbols

k	First order rate constant for removal from top soil	[d^{-1}]	Equation 33
Facc	Fraction accumulated in one year	[-]	

The maximum concentration in soil following the last application in year 10 is calculated with Equation 36.

$$Csoil_{10} = Csoil_{\max\_1} \times \left(1 + \sum_{n=1}^{9} Facc^{n}\right)$$ **Equation 36**

Explanation of symbols

$Csoil_{max\_1}$	Maximum concentration in soil in year 1	[$mg.kg_{wwt}^{-1}$]	Equation 34
Facc	Fraction accumulated in one year	[-]	Equation 35
$Csoil_{10}$	Maximum concentration in soil in year 10	[$mg.kg_{wwt}^{-1}$]	

3.6.2.8 Time-weighted average concentration in soil

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

$$TWACsoil(t) = Csoil_{10} \times \frac{\left(1 - e^{(-k \times t)}\right)}{(k \times t)}$$ **Equation 37**

Explanation of symbols

$Csoil_{10}$	Maximum concentration in soil in year 10	[$mg.kg_{wwt}^{-1}$]	Equation 36
k	First order rate constant for removal from top soil	[d^{-1}]	Equation 33
t	Time period	[d]	Soil: 30 Secondary poisoning: 180 Humans via environment: 180
TWACsoil(t)	Time weighted average concentration in soil, over a period t	[$mg.kg_{wwt}^{-1}$]	

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:

$$TWACsoil(t) = Csoil_{\max\_1} \times \frac{\left(1 - e^{(-k \times t)}\right)}{(k \times t)}$$ **Equation 38**

Explanation of symbols

$Csoil_{max\_1}$	Maximum concentration in soil in year 1	[mg.kg$_{wwt}^{-1}$]	Equation 34
k	First order rate constant for removal from top soil	[d^{-1}]	Equation 33
t	Time period	[d]	Soil: 30 Secondary poisoning: 180 Humans via environment: 180
TWACsoil(t)	Time weighted average concentration in soil, over a period t	[mg.kg$_{wwt}^{-1}$]	

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 39), rather than the 28 days used by default by FOCUS (2003).

$$Clocal_{soil} = TWACsoil(30d)$$ **Equation 39**

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.

$$Clocal_{soil,secondarypoisoning} = TWACsoil(180d)$$ **Equation 40**

$$Clocal_{soil,humans\ via\ env} = TWACsoil(180d)$$ **Equation 41**

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 42.

$$Ksoil - water = Fair_{soil} \times Kair - water + Fwater_{soil} + Fsolid_{soil} \times \frac{Kpsoil}{1000} \times RHOsolid$$ **Equation 42**

Where:

$$Kp_{soil} = K_{OC} \times Foc_{soil}$$ **Equation 43**

$$K_{air-water} = \frac{HENRY}{R \times TEMP}$$ **Equation 44**

$$HENRY = \frac{VP(TEMP_{env}) \times MOLW}{SOL(TEMP_{env})}$$ **Equation 45**

Explanation of symbols

VP(TEMPenv)	Vapour Pressure at environmental temperature (12 °C)	[Pa]	Equation 47
SOL(TEMP$_{env}$)	Solubility in water at environmental temperature (12 °C)	[mg.L^{-1}]	Equation 46
MOLW	Molecular weight	[g.mol^{-1}]	User input
R	Gas constant	[Pa.m^3.mol^{-1}.K^{-1}]	8.314
TEMP	Temperature at the air-water interface	[K]	285
K$_{OC}$	Partition coefficient organic carbon -water	[L.kg^{-1}]	User input
Foc$_{soil}$	Fraction organic carbon in the soil	[-]	0.02
Fair$_{soil}$	Fraction air in soil	[-]	0.2
Fwater$_{soil}$	Fraction water in soil	[-]	0.2
Fsolid$_{soil}$	Fraction solid in soil	[-]	0.6
RHOsolid	Bulk density of solids	[kg.m^{-3}]	2500
HENRY	Henry's law constant	[Pa.m^3.mol^{-1}]	
K$_{air-water}$	Air-water partitioning coefficient	[-]	
Kpsoil	Solids-water partition coefficient in soil	[L.kg^{-1}]	
K$_{soil-water}$	Soil-water partitioning coefficient	[m^3.m^{-3}]	

The water solubility and vapour pressure are converted from test temperature to environmental temperature using Equation 46 and Equation 47, respectively.

$$SOL(TEMP_{env}) = SOL(TEMP_{test}) \times e^{\left(\left(\frac{H_{0solut}}{R} \times \left(\frac{1}{273 + TEMP_{test}} - \frac{1}{273 + 12}\right)\right)\right)}$$ **Equation 46**

$$VP(TEMP_{env}) = VP(TEMP_{test}) \times e^{\left(\left(\frac{H_{0vapor}}{R} \times \left(\frac{1}{273 + TEMP_{test}} - \frac{1}{273 + 12}\right)\right)\right)}$$ **Equation 47**

Explanation of symbols

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

$SOL(TEMP_{env})$	Solubility in water at environmental temperature (12 °C)	[mg.L^{-1}]
$VP(TEMP_{env})$	Vapour Pressure at environmental temperature (12 °C)	[Pa]

The concentration in porewater is calculated using Equation 48. 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.

$$C_{soil\ porewater} = \frac{C_{soil\ wwt} \times \mathrm{RHOsoil}}{K\mathrm{soil\text{-}water} \times 1000}$$ **Equation 48**

Explanation of symbols

$K_{soil\text{-}water}$	Soil-water partitioning coefficient	[mg.m^{-3}]	Equation 42
RHOsoil	Bulk density of wet soil	[kg.m^{-3}]	1700
$C_{soil\ wwt}$	Concentration in soil (wet weight) as a 180d time weighted average	[mg.kg$_{wwt}^{-1}$]	Equation 40
$C_{soil\ porewater}$	Concentration in soil porewater	[mg.L^{-1}]	

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^3 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^2) waterbody will have a volume of 3 x 10^5 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 25. For the LET 'Default' assessment, the spray drift value for one application to 'fruit (late)' was selected (see Table 20). 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 24 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 24: 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
Vines, early applications	3	2.7	2.5	2.8	2.5	2.4	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	1.5
Spray to bare soil / pre-emergent use	1	2.8	2.4	2.0	1.9	1.8	1.6	1.6	1.5
Arable crops	1	2.8	2.4	2.0	1.9	1.8	1.6	1.6	1.5
Vegetable crops	1	2.8	2.4	2.0	1.9	1.8	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
Hand applications (crop > 50 cm)	3	8.0	7.1	6.9	6.6	6.6	6.4	6.2	6.2
Fruit (late)	3	15.7	12.1	11.0	10.1	9.7	9.2	9.1	8.7
Hops	3	19.3	17.7	15.9	15.4	15.1	14.9	14.6	13.5
Fruit (early)	3	29.2	15.5	24.0	23.6	23.1	22.8	22.7	22.2
Aerial application	3	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 25).

Table 25: 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**
Arable and vegetable crops: (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
Fruit (late) Citrus, olives, pome / stone fruit (late)	3	15.7	12.1	11.0	10.1	9.7	9.2	9.1	8.7
Fruit (early)	3	29.2	25.5	24.0	23.6	23.1	22.8	22.7	22.2

Crop	Distance crop-water (m)	% drift (Number of applications per season)							
		1	2	3	4	5	6	7	>7
pome / stone fruit, (early)									
vines, early applications	3	2.7	2.5	2.5	2.5	2.4	2.3	2.3	2.3
vines, late applications	3	8.0	7.1	6.9	6.6	6.6	6.4	6.2	6.2
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 49.

$$Input\ Drift\ = \frac{AR\ \times\ Drift\ \%}{1000}$$ **Equation 49**

Explanation of symbols

AR	Equivalent application rate for co-formulant	[g.ha^{-1}]	User input
Drift %	Drift percentage	[%]	Table 25
Input Drift	Input *via* single drift event	[mg.m^{-2}]	

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 27.

The concentration in soil after the final application is calculated in Equation 50 and only includes biodegradation as a removal process (i.e. leaching and volatilisation are not included).

$$Eq\ Rate\ Runoff\ Final = Soil\ Loading\ \times \frac{1 - e^{\left((-Napp\ \times\ App\ Int\ \times \frac{ln(2)}{\mathrm{DT50soil}})\right)}}{1 - e^{\left((-App\ Int\ \times \frac{ln(2)}{\mathrm{DT50soil}})\right)}}$$ **Equation 50**

Explanation of symbols

DT_{50}soil	Half-life of the co-formulant in soil	[days]	User input
App Int	Interval between applications	[days]	User input
Napp	Number of application events	[-]	User input

Soil Loading	Soil loading of the co-formulant	[g.ha^{-1}]	Equation 27
Eq Rate Runoff Final	Equivalent rate for runoff after the last treatment	[g.ha^{-1}]	

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 51.

$$Eq\ Rate\ Runoff\ Event = Eq\ Rate\ Runoff\ Final \times e^{\left((-4 \times \frac{ln(2)}{\mathrm{DT50soil}})\right)}$$ **Equation 51**

Explanation of symbols

DT_{50}soil	Half-life of the co-formulant in soil	[days]	User input
Eq Rate Runoff Final	Equivalent rate for runoff after the last treatment	[g.ha^{-1}]	Equation 50
Eq Rate Runoff Event	Equivalent rate for runoff at the time of the runoff event	[g.ha^{-1}]	

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 26. For the LET 'Default' assessment parameterisation, the worst-case runoff value of 5% for 'North Europe, Oct – Feb' has been assumed (see Table 20), giving a worst-case assessment of exposure via runoff. The region and season of application can be defined by selecting 'Refinement option'.

Table 26: 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 52 where the waterbody is assumed to have an area equivalent to one tenth of the field from which it receives runoff or drainage water.

$$Input\ Runoff = \frac{Eq\ Rate\ Runoff\ Event \times Runoff\ \% \times FW\ Ratio}{1000}$$ **Equation 52**

Explanation of symbols

Eq Rate Runoff Event	Equivalent rate for runoff at the time of the runoff event	[g.ha^{-1}]	Equation 51
Runoff %	Runoff percentage (related to soil residue)	[%]	Default: 5%

			Refinement: Table 26
FW Ratio	Ratio of field to waterbody	[-]	10
Input Runoff	Input via runoff	[mg.m^{-2}]	

Equation 52 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 53).

$$Fwaterphase_{runoff} = \frac{Water\ Depth}{Water\ Depth + (Eff\ Sed\ Depth \times RHOsed \times OC \times \frac{K_{OC}}{100})}$$ **Equation 53**

Explanation of symbols

Water Depth	Depth of the surface water	[cm]	30
Eff Sed Depth	Effective sediment depth of the surface water	[cm]	1
RHOsed	Sediment bulk density	[kg.L^{-1}]	0.8
OC	Sediment organic carbon content	[%]	5
K_{OC}	Soil sorption constant related to org carbon	[L.kg^{-1}]	User input
Fwater phase$_{runoff}$	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 54 and Equation 55, respectively.

$$Input\ Runoff_{sw} = Input\ Runoff \times Fwaterphase_{runoff}$$ **Equation 54**

$$Input\ Runoff_{sed} = Input\ Runoff \times (1 - Fwaterphase_{runoff})$$ **Equation 55**

Explanation of symbols

Fwater phase$_{runoff}$	Fraction of substance entering in water phase *via* runoff	[-]	Equation 53
Input Runoff	Total input *via* runoff	[mg.m^{-2}]	Equation 52
Input Runoff$_{sw}$	Runoff input *via* water phase	[mg.m^{-2}]	
Input Runoff$_{sed}$	Runoff input *via* sediment phase	[mg.m^{-2}]	

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.

$$Input_{sw}(app) = Input\ Drift$$ **Equation 56**

$$Input_{sed}(app) = 0$$ **Equation 57**

Explanation of symbols

Input Drift	Input *via* a single drift event	[mg.m^{-2}]	Equation 49
Input$_{sw}$(app)	Input into the water phase, on the day of application	[mg.m^{-2}]	
Input$_{sed}$(app)	Input into the sediment phase, on the day of application	[mg.m^{-2}]	

$$Input_{sw}(storm) = Input\ Runoff_{sw}$$ **Equation 58**

$$Input_{sed}(storm) = Input\ Runoff_{sed}$$ **Equation 59**

Explanation of symbols

Input Runoff$_{sw}$	Runoff input *via* water phase	[mg.m^{-2}]	Equation 54
Input Runoff$_{sed}$	Runoff input *via* sediment phase	[mg.m^{-2}]	Equation 55
Input$_{sw}$(storm)	Input into the water phase, on the day of erosion/drainage/runoff event	[mg.m^{-2}]	
Input$_{sed}$(storm)	Input into the sediment phase, on the day of erosion/drainage/runoff event	[mg.m^{-2}]	

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.

$$Mass_{sw}(0) = Input_{sw}(app) = Input\ Drift$$ **Equation 60**

$$Mass_{sed}(0) = Input_{sed}(app) = 0$$ **Equation 61**

Explanation of symbols

Input Drift	Input *via* single drift event	[mg.m^{-2}]	Equation 49
Input$_{sw}$(app)	Input into the water phase, on the day of application	[mg.m^{-2}]	
Input$_{sed}$(app)	Input into the sediment phase, on the day of application	[mg.m^{-2}]	
Mass$_{sw}$ (0)	Substance mass in the surface water on day *0*	[mg.m^{-2}]	
Mass$_{sed}$(0)	Substance mass in the sediment on day *0*	[mg.m^{-2}]	

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 62 and Equation 63.

$$Mass_{sw}\ int_{available}(0) = \frac{\mathrm{Mass_{sw}\ int(0)}}{\mathrm{Dist\ Coeff}}$$ **Equation 62**

$$Mass_{sw}\ int_{unavailable}(0) = \mathrm{Mass_{sw}\ int(0)} - \mathrm{Mass_{sw}}\ int_{\mathrm{available}}(0)$$ **Equation 63**

Explanation of symbols

$Mass_{sw}int(0)$	Temporary substance mass in the surface water at the end of day *0*	[mg.m^{-2}]	Equation 60
Dist Coeff	Distribution coefficient	[-]	1.5 (on day 0)
$Mass_{sw}int_{available}(0)$	Temporary substance mass in the surface water at the end of day 0 that is available for sorption	[mg.m^{-2}]	
$Mass_{sw}int_{unavailable}(0)$	Temporary substance mass in the surface water at the end of day 0 that is not available for sorption	[mg.m^{-2}]	

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

$$Mass_{sw}\ (end\_day\_0) = Mass_{sw}\ int_{\ unavailable}\ (0) + (Mass_{sw}\ int_{\ available}(0) + Mass_{sed}\ int(0)) \times Fwaterphase_{runoff}$$ **Equation 64**

$$Mass_{sed}(end\_day\_0) = Mass_{sw}\ int(0) + Mass_{sed}\ int(0) - Mass_{sw}(end\_day\_0)$$ **Equation 65**

Explanation of symbols

$Mass_{sw}int(0)$	Temporary substance mass in the surface water at the end of day *0*	[mg.m^{-2}]	Equation 60
$Mass_{sed}int(0)$	Temporary substance mass in the sediment at the end of day *0*	[mg.m^{-2}]	Equation 61
Fwater phase$_{runoff}$	Fraction of compound entering in water phase *via* runoff	[-]	Equation 53
$Mass_{sw}int_{available}(0)$	Temporary substance mass in the surface water at the end of day 0 that is available for sorption	[mg.m^{-2}]	Equation 62
$Mass_{sw}int_{unavailable}(0)$	Temporary substance mass in the surface water at the end of day 0 that is not available for sorption	[mg.m^{-2}]	Equation 63
$Mass_{sw}$(end_day_0)	Substance mass in the surface water at the end of day *0*	[mg.m^{-2}]	

$Mass_{sed}$(end_day_0)	Substance mass in the sediment at the end of day *0*	[mg.m^{-2}]

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.

$$Mass_{sw}\ int(i) = Mass_{sw}(i-1) \times e^{\left(\left(\frac{-ln(2)}{\mathrm{DT50sw}}\right)\right)} + Input_{sw}(i) \quad \textbf{Equation 66}$$

$$Mass_{sed}\ int(i) = Mass_{sed}(i-1) \times e^{\left(\left(\frac{-ln(2)}{\mathrm{DT50sed}}\right)\right)} + Input_{sed}(i) \quad \textbf{Equation 67}$$

Explanation of symbols

$Mass_{sw}$(*i*-1)	Substance mass in the surface water on day *i-1*	[mg.m^{-2}]	If i= 1 then: Equation 64 Otherwise: Equation 70
$Mass_{sed}$(*i*-1)	Substance mass in the sediment on day *i-1*	[mg.m^{-2}]	If i= 1 then: Equation 65 Otherwise: Equation 71
$Input_{sw}$(*i*)	Input into the water phase, on day i	[mg.m^{-2}]	Equation 49 and Equation 58
$Input_{sed}$(*i*)	Input into the sediment phase, on day i	[mg.m^{-2}]	Equation 59
$DT_{50}sw$	Half-life of the substance in surface water	[days]	User input
$DT_{50}sed$	Half-life of the substance in sediment	[days]	User input
$Mass_{sw}int$(*i*)	Temporary substance mass in the surface water on day *i*	[mg.m^{-2}]	
$Mass_{sed}int$(*i*)	Temporary substance mass in the sediment on day *i*	[mg.m^{-2}]	

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.

$$Mass_{sw}\ int_{available}(i) = \frac{\mathrm{Mass_{sw}\ int}(i)}{\mathrm{Dist\ Coeff}} \quad \textbf{Equation 68}$$

$$Mass_{sw}\ int_{unavailable}(i) = \mathrm{Mass_{sw}\ int}(i) - Mass_{sw}\ int_{\mathrm{available}}(i) \quad \textbf{Equation 69}$$

Explanation of symbols

$Mass_{sw}int(i)$	Temporary substance mass in the surface water on day *i*	[mg.m^{-2}]	Equation 66
Dist Coeff	Distribution coefficient	[-]	Before the runoff event = 1.5 During and after the runoff event = 1
$Mass_{sw}int_{available}(i)$	Temporary substance mass in the surface water on day *i* that is available for sorption	[mg.m^{-2}]	
$Mass_{sw}int_{unavailable}(i)$	Temporary substance mass in the surface water on day *i* that is not available for sorption	[mg.m^{-2}]	

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:

$$Mass_{sw}(i) = Mass_{sw}\ int\ unavailable(i) + (Mass_{sw}\ int\ available(i) + Mass_{sed}\ int(i)) \times Fwaterphase_{runoff}$$ **Equation 70**

$$Mass_{sed}(i) = Mass_{sw}\ int(i) + Mass_{sed}\ int(i) - Mass_{sw}(i)$$ **Equation 71**

Explanation of symbols

$Mass_{sw}int(i)$	Temporary substance mass in the surface water on day *i*	[mg.m^{-2}]	Equation 66
$Mass_{sed}int(i)$	Temporary substance mass in the sediment on day *i*	[mg.m^{-2}]	Equation 67
$Fwater\ phase_{runoff}$	Fraction of substance entering in water phase via runoff	[-]	Equation 53
$Mass_{sw}int_{available}(i)$	Temporary substance mass in the surface water on day *i* that is available for sorption	[mg.m^{-2}]	Equation 68
$Mass_{sw}int_{unavailable}(i)$	Temporary substance mass in the surface water on day *i* that is not available for sorption	[mg.m^{-2}]	Equation 69
$Mass_{sw}(i)$	Substance mass in the surface water on day *i*	[mg.m^{-2}]	
$Mass_{sed}(i)$	Substance mass in the sediment on day *i*	[mg.m^{-2}]	

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.

$$Clocal_{SW}(i) = \frac{Mass_{SW}int(i) \times 100}{Water\ Depth}$$ **Equation 72**

$$Clocal_{SED}(i) = \frac{Mass_{sed}int(i) \times 100}{Sed\ Depth \times RHOsed}$$ **Equation 73**

Explanation of symbols

Mass$_{sw}$int(i)	Temporary substance mass in the surface water on day *i*	[mg.m^{-2}]	Equation 66
Mass$_{sed}$int(i)	Temporary substance mass in the sediment on day *i*	[mg.m^{-2}]	Equation 67
Water Depth	Depth of the surface water	[cm]	30
Sed Depth	Sediment depth	[cm]	5
RHOsed	Sediment bulk density	[kg.L^{-1}]	0.8
Clocal$_{SW}$ (i)	Surface water concentration on day *i*	[µg.L^{-1}]	
Clocal$_{SED}$ (i)	Sediment concentration on day *i*	[µg.kg$_{dwt}^{-1}$]	

Daily local concentrations in surface water and sediment are calculated using Equation 72 and Equation 73, respectively. The maximum local concentrations in surface water and sediment are calculated using Equation 74 and Equation 75, respectively, and then used in the risk characterisation ratios for surface water and sediment (see Section 3.6.6).

$$Clocal_{SW} = Maximum\ Clocal_{SW}(i)$$ **Equation 74**

Explanation of symbols

Clocal$_{SW}$ (i)	Surface water concentration on day *i*	[µg.L^{-1}]	Equation 72
Clocal$_{sw}$	Maximum local freshwater concentration	[µg.L^{-1}]	

$$Clocal_{sed\ (dwt)} = Maximum\ Clocal_{SED}(i)$$ **Equation 75**

Explanation of symbols

Clocal$_{SED}$ (i)	Sediment concentration on day *i*	[µg.kg $_{dwt}^{-1}$]	Equation 73
Clocal$_{sed\ (dwt)}$	Maximum local freshwater sediment concentration (dry weight)	[µg.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 74and Equation 75. 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 76 and Equation 77 will be worst-case.

$$Clocal_{marine\ water} = \frac{Clocal_{sw}}{10}$$ **Equation 76**

$$Clocal_{marine\ sed\ (dwt)} = \frac{Clocal_{sed\ (dwt)}}{10}$$ **Equation 77**

Explanation of symbols

$Clocal_{sw}$	Maximum local freshwater concentration	[µg.L^{-1}]	Equation 74
$Clocal_{sed\ (dwt)}$	Maximum local freshwater sediment concentration (dry weight)	[mg.kg$_{dwt}^{-1}$]	Equation 75
$Clocal_{marine\ water}$	Local marine water concentration	[µg.L^{-1}]	
$Clocal_{marine\ sed\ (dwt)}$	Local marine sediment concentration (dry weight)	[mg.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 78and Equation 79.

$$Clocal\_24TWA_{sw}(i) = \frac{(Clocal_{sw}(i-1) + Clocal_{sw}(i))}{2}$$ **Equation 78**

$$Clocal\_24TWA_{SED}(i) = \frac{(Clocal_{SED}(i-1) + Clocal_{SED}(i))}{2}$$ **Equation 79**

Explanation of symbols

$Clocal_{SW}$ *(i-1)*	Surface water concentration on day *i-1*	[µg.L^{-1}]	Equation 72
$Clocal_{SED}$ *(i-1)*	Sediment concentration on day *i-1*	[µg.kg$_{dwt}^{-1}$]	Equation 73
$Clocal_{SW}$ *(i)*	Surface water concentration on day *i*	[µg.L^{-1}]	Equation 72
$Clocal_{SED}$ *(i)*	Sediment concentration on day *i*	[µg.kg$_{dwt}^{-1}$]	Equation 73
$Clocal\_24TWA_{SW}$ *(i)*	24 hour averaged surface water concentration on day *i*	[µg.L^{-1}]	
$Clocal\_24TWA_{SED}$ *(i)*	24 hour averaged sediment concentration on day *i*	[µg.kg$_{dwt}^{-1}$]	

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:

$$TWAC_{sw}(t) = \frac{\left(\sum_{i=imax+1}^{imax+t} Clocal\_24TWA_{sw}(i)\right)}{t}$$ **Equation 80**

$$TWAC_{SED}(t) = \frac{\left(\sum_{i=imax+1}^{imax+t} Clocal\_24TWA_{SED}(i)\right)}{t}$$ **Equation 81**

Explanation of symbols

Clocal_24TWA$_{SW}$ (i)	24 hour averaged surface water concentration on day *i*	[µg.L^{-1}]	Equation 78
Clocal_24TWA$_{SED}$ (i)	24 hour averaged sediment concentration on day *i*	[µg.kg$_{dwt}^{-1}$]	Equation 79
i_{max}	Day of the maximum surface water or sediment concentration	[d]	
t	Time period	[d]	Secondary poisoning: 21 Humans via environment: 21
TWAC$_{sw}$(t)	Time weighted average concentration in surface water, over a period t	[µg.L^{-1}]	
TWAC$_{SED}$(t)	Time weighted average concentration in sediment, over a period t	[µg.kg$_{dwt}^{-1}$]	

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 83.

$$Clocal_{sw,secondary\ poisoning} = TWAC_{SW}(21d)$$ **Equation 82**

$$Clocal_{sw,HvE,fish} = TWAC_{SW}(21d)$$ **Equation 83**

The corresponding local marine water concentration used for the marine water secondary poisoning assessment is calculated using Equation 84.

$$Clocal_{mw,secondary\ poisoning} = \frac{Clocal_{sw\ (21d)}}{10}$$ **Equation 84**

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_{OW} ≥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 87 to Equation 94. If experimental data are not available, the BCF for fish can be predicted from the relationship between K_{OW} and BCF derived by Veith et al. (1979). For substances with a log K_{OW} of 2 to 6, the BCF in fish is estimated using Equation 85.

$$log\ BCF_{fish} = 0.85 \times log\ Kow - 0.70$$ **Equation 85**

For substances with a log K_{ow} higher than 6, Equation 86 is used:

$$log\ BCF_{fish} = -0.20 \times log\ Kow^2 + 2.74 \times log\ Kow - 4.72$$ **Equation 86**

Explanation of symbols

Kow	Octanol-water partition coefficient	[-]	User input
BCF_{fish}	Bioconcentration factor for fish on wet weight basis	[L.kg $_{wet\ fish}^{-1}$]	

This approach is considered appropriate to estimate BCF_{fish} when the log K_{OW} is between 1 and 10. If the log K_{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_{OW} with default BMF_1 values summarised in Table 27.

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 27). When measured BCF values are available, these are used to determine the BMF values.

Table 27: Default BMF values for organic substances (ECHA R16 guidance R.16.5.3.5, (2016))

log K_{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 $PEC_{surface\ water}$, bioconcentration in fish and the biomagnification factor (Equation 87). This is the standard approach in the assessment of active substances in PPP.

$$PEC_{\ oral,\ predator} = PEC_{sw} \times BCF_{fish} \times BMF_1 \qquad \textbf{Equation 87}$$

Where:

$$PEC_{sw} = \frac{Clocal_{sw,secondary\ poisoning}}{1000} + PECregional_{sw(dissolved)} \qquad \textbf{Equation 88}$$

Explanation of symbols

PEC_{sw}	PEC in surface water at local scale	[mg.L^{-1}]	
$Clocal_{sw,secondary\ poisoning}$	21-day TWA surface water concentration	[µg.L^{-1}]	Equation 82
$PECregional_{sw\ (dissolved)}$	Surface 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 85 and Equation 86)
BMF_1	Biomagnification factor in fish	[-]	Table 27
$PEC_{oral,\ predator}$	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 87 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 89).

$$PEC_{oral,\ predator} = 0.5 \times (PEC_{sw} + PECregional_{sw(dissolved)}) \times BCF_{fish} \times BMF$$ **Equation 89**

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 90), in analogy to the approach used for the freshwater environment.

$$PEC_{oral,\ marinepredator} = PEC_{mw} \times BCF_{fish} \times BMF_1$$ **Equation 90**

Where:

$$PEC_{mw} = \frac{Clocal_{mw,secondary\ poisoning}}{1000} + PECregional_{mw(dissolved)}$$ **Equation 91**

Explanation of symbols

PEC_{mw}	PEC in marine water at local scale	[mg.L^{-1}]	
$Clocal_{mw,\ secondary\ poisoning}$	21-day TWA marine water concentration	[µg.L^{-1}]	Equation 84
$PECregional_{mw\ (dissolved)}$	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 85 and Equation 86)
BMF_1	Biomagnification factor in fish	[-]	Table 27
$PEC_{oral,\ marine\ predator}$	Predicted environmental concentration in food	[mg.kg$_{wet\ fish}^{-1}$]	

Equation 91 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 92).

$$PEC_{oral,\ marinepredator} = 0.5 \times (PEC_{mw} + PECregional_{mw\ (dissolved)}) \times BCF_{fish} \times BMF_1$$ **Equation 92**

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 93).

$$PEC_{oral,\ top\ predator} = PEC_{mw} \times BCF_{fish} \times BMF_1 \times BMF_2$$ **Equation 93**

Explanation of symbols

PEC_{mw}	21-day TWA PEC in marine water at local scale	[mg.L^{-1}]	Equation 91
BCF_{fish}	Bioconcentration factor for fish on wet weight basis	[L.kg $_{\text{wet fish}}^{-1}$]	Measured or estimated from log K_{ow} (Equation 85 and Equation 86)
BMF_1	Biomagnification factor in fish	[-]	Table 27
BMF_2	Biomagnification factor in predator	[-]	Table 27
$PEC_{oral,\ marine\ predator}$	Predicted environmental concentration in food	[mg.kg$_{\text{wet fish}}^{-1}$]	

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 94).

$$PEC_{oral,toppredator} = (0.1 \times PEC_{mw} + 0.9 \times PECregional_{mw_{(dissolved)}}) \times BCF_{fish} \times BMF_1 \times BMF_2$$

Equation 94

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 96 and Equation 100. If experimental data are not available, bioconcentration in earthworms can be estimated according to Equation 95 described by Jager (1998).

$$BCF_{earthworm} = \frac{(0.84 + 0.012 \times K_{ow})}{RHO_{earthworm}}$$

Equation 95

Explanation of symbols

$RHO_{earthworm}$	Earthworm density	[kg_{wwt}.L^{-1}]	1
Kow	Octanol-water partition coefficient	[-]	User input
$BCF_{earthworm}$	Bioconcentration factor for earthworms on wet weight basis	[L.kg$_{\text{wet earthworm}}^{-1}$]	

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 PECoral$_{\text{predator}}$ is calculated using Equation 96.

$$PEC_{oralpredator} = C_{earthworm} = \frac{BCF_{earthworm} \times PEC_{porewater,sec.\ poisoning} + PEC_{soil,sec.\ poisoning} \times F_{gut} \times CONV_{soil}}{1 + F_{gut} \times CONV_{soil}}$$

Equation 96

Where:

$$CONV_{soil} = \frac{RHO_{soil}}{F_{solid} \times RHO_{solid}}$$ **Equation 97**

$$PEC_{porewater,sec.\ poisoning} = C_{soil\ porewater} + \left(\left(\frac{PEC_{regional\ agric.\ soil} \times RHO_{soil}}{Ksoilwater \times 1000} \right) \right)$$ **Equation 98**

$$PEC_{soil,sec.\ poisoning} = TWAC_{soil(180d)} + PEC_{regional\ agric.\ soil}$$ **Equation 99**

Explanation of symbols

$BCF_{earthworm}$	Bioconcentration factor for earthworms on wet weight basis	[L.kg$_{wet\ earthworm}^{-1}$]	Measured or estimated from log K_{ow} (Equation 95)
$PEC_{porewater,\ sec.\ poisoning}$	Predicted environmental concentration in porewater at local scale for secondary poisoning	[mg.L^{-1}]	Equation 98
$PEC_{soil,\ sec.\ poisoning}$	Predicted environmental concentration in soil at local scale for secondary poisoning	[mg.kg$_{wwt}^{-1}$]	Equation 99
F_{gut}	Fraction of gut loading in worm	[kg$_{dwt}$.kg$_{wwt}^{-1}$]	0.1
$CONV_{soil}$	Conversion factor for soil concentration wet-dry weight soil	[kg$_{wwt}$.kg$_{dwt}^{-1}$]	Equation 97
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 48
$PEC_{regional\ agric.\ soil}$	Regional predicted environmental concentration in agricultural soil	[mg.kg$_{wwt}^{-1}$]	Input (calculated outside LET) otherwise assumed to be 0
$K_{soil\text{-}water}$	Soil-water partitioning coefficient	[mg.m^{-3}]	Equation 42
$TWAC_{soil(180d)}$	Local concentration in soil over a 180d time weighted average period	[mg.kg$_{wwt}^{-1}$]	Equation 40
$C_{earthworm}$	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 96 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 100).

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

$$PEC_{oral,predator}(earthworm) = C_{earthworm} = \frac{\left(\begin{array}{c} BCF_{earthworm} \times 0.5 \times (PEC_{porewater,sec\,poisoning} + PECregional_{agric.\,soil\,porewater}) \\ + 0.5 \times (PEC_{soil,sec\,poisoning} + PECregional_{agric.\,soil}) \times F_{gut} \times CONV_{soil} \end{array}\right)}{1 + F_{gut} \times CONV_{soil}}$$

Equation 100

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^2/d and receptor point 10 metre downwind and estimates the concentration in air 10 meters downwind from an agricultural field.

$$DOSE_{pest} = \frac{AR}{A_{field} \times 1000}$$ **Equation 101**

Explanation of symbols

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

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^2 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 28.

Table 28: 24-hour source strengths for field use of pesticides (RIVM, VROM, VWS (2002))

Vapour pressure at 25 °C (Pa)	24 hour averaged source strength ($kg.m^{-2}.d^{-1}$)
≥ 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 28 represent an application density of 1 kg per m^2 and are converted to the expected 24-hour emission strength following application using Equation 102.

$$E_{field,air,24\,h} = \frac{Estd_{field,air,24\,h}}{1} \times DOSE_{pest}$$ **Equation 102**

Explanation of symbols

$Estd_{field,air,24\,h}$	Standard 24-hour emission strength of the field	[$kg.m^{-2}.d^{-1}$]	Table 28
1	Standard dose of source strength	[$kg.m^{-2}$]	
$DOSE_{pest}$	Single dose of pesticide	[$kg.m^{-2}$]	Equation 101
$E_{field,air,24\,h}$	24-hour emission strength of the field	[$kg.m^{-2}.d^{-1}$]	

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 103.

$$C_{field,air,24\,h} = \frac{E_{field,air,24\,h}}{1} \times Cstd_{field,air,1\,h}$$ **Equation 103**

Explanation of symbols

$E_{field,air,24\,h}$	24-hour emission strength of the field	[$kg.m^{-2}.d^{-1}$]	Equation 102
1	Standard source strength	[$kg.m^{-2}.d^{-1}$]	
$Cstd_{field,air,1\,h}$	1 hour averaged concentration at 10 metres downwind of field with a standard source strength	[$kg.m^{-3}$]	1.28×10^{-4}
$C_{field,air,24\,h}$	24 hour averaged concentration at 10 metres downwind of field	[$kg.m^{-3}$]	

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 104.

$$C_{daily,air} = \left(C_{field,air,24\,h} \times 1000000\right) + PECregional_{air}$$ **Equation 104**

Explanation of symbols

$C_{field,air,24\ h}$	24-hour averaged concentration at 10 metres downwind of field	[kg.m^{-3}]	Equation 103
$PECregional_{air}$	Regional PEC in air	[mg.m^{-3}]	Input (calculated outside LET) otherwise assumed to be 0
$C_{daily,air}$	Daily concentration in air	[mg.m^{-3}]	

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

If the General Population, systemic effects, long term inhalation DNEL is in mg/m^3, the daily dose via inhalation is calculated using Equation 105. 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 106.

$$DOSE_{air} = C_{daily,air}$$ **Equation 105**

$$DOSE_{air} = \frac{C_{daily,air} \times F_{resp} \times IH_{air}}{BW} \times \frac{BIO_{inh}}{BIO_{oral}}$$ **Equation 106**

Explanation of symbols

$C_{daily,air}$	Daily concentration in air	[mg.m^{-3}]	Equation 104
F_{resp}	Respirable fraction of inhaled substance	[-]	1
IH_{air}	Daily intake of air	[m^3.d^{-1}]	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}] or [mg.kg^{-1}.d^{-1}]	

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 107.

$$PEClocal_{gw\_dw} = \left(\frac{TWACsoil\ (180d) \times RHO_{soil}}{K_{soil-water} \times 1000}\right) + PECregional_{porewater} \qquad \textbf{Equation 107}$$

Explanation of symbols

TWACsoil(180d)	Local concentration in soil (wet weight) as a 180d time weighted average	[mg.kg$_{wwt}^{-1}$]	Equation 41
RHOsoil	Bulk density of wet soil	[kg.m^{-3}]	1700
$K_{soil\text{-}water}$	Soil-water partitioning coefficient	[m^3.m^{-3}]	Equation 42
$PECregional_{porewater}$	Regional PEC in porewater	[mg.L^{-1}]	Input (calculated outside LET) otherwise assumed to be 0
$PEClocal_{gw\_dw}$	Predicted environmental concentration in soil porewater (drinking water)	[mg.L^{-1}]	

The local concentration in drinking water is estimated using Equation 108 and the purification factor is calculated using Equation 109.

$$PEClocal_{sw\_dw} = \left(\frac{Clocal_{sw\ max}}{1000}\right) \times F_{pur} \qquad \textbf{Equation 108}$$

Explanation of symbols

$Clocal_{sw\ max}$	Maximum local freshwater concentration	[µg.L^{-1}]	Equation 74
Fpur	Purification factor for surface water	[-]	Equation 109

$PEClocal_{sw\_dw}$	Predicted environmental concentration in surface water (drinking water)	[mg.L^{-1}]	

$$F_{pur} = max(Fsys1_{pur}, Fsys2_{pur})$$ **Equation 109**

Explanation of symbols

$Fsys1_{pur}$	Purification factor system 1	[-]	Table 29
$Fsys2_{pur}$	Purification factor system 2	[-]	Table 29
F_{pur}	Purification factor for surface water	[-]	

Table 29: Purification factors (EU-TGD, 2003b)

Treatment process	Log Kow			Henry's Law constant (Pa.m^3.mol^{-1})		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 110.

$$CONC_{drw,L} = max(PEClocal_{gw\_dw}, PEClocal_{sw\_dw})$$ **Equation 110**

Explanation of symbols

$PEClocal_{gw\_dw}$	Predicted environmental concentration in soil porewater (drinking water)	[mg.L^{-1}]	Equation 107
$PEClocal_{sw\_dw}$	Predicted environmental concentration in surface water (drinking water)	[mg.L^{-1}]	Equation 108
$CONC_{drw,\,L}$	Local concentration in drinking water	[mg.L^{-1}]	

If regional PECs are not available then the daily dose via drinking water is calculated using Equation 111.

$$DOSE_{drw} = \frac{CONC_{drw,L} \times IH_{drw}}{BW}$$ **Equation 111**

Explanation of symbols

$CONC_{drw,L}$	Local concentration in drinking water	[mg.L^{-1}]	Equation 110
IH_{drw}	Daily intake of drinking water	[L.d^{-1}]	2
BW	Bodyweight	[kg]	60
$DOSE_{drw}$	Daily dose via drinking water	[mg.kg^{-1}.d^{-1}]	

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 112.

$$CONC_{drw,R} = max\left(PECregional_{soil\ porewater}, \left(PECregional_{sw} \times F_{pur}\right)\right) \quad \textbf{Equation 112}$$

Explanation of symbols

$PECregional_{soil\ porewater}$	Regional predicted environmental concentration in agricultural soil porewater	[mg.L^{-1}]	Input (calculated outside LET) otherwise assumed to be 0
$PECregional_{sw}$	Regional predicted environmental concentration in surface water	[mg.L^{-1}]	Input (calculated outside LET) otherwise assumed to be 0
F_{pur}	Purification factor for surface water	[-]	Equation 109
$CONC_{drw,R}$	Regional concentration in drinking water	[mg.L^{-1}]	

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:

$$DOSE_{drw} = \frac{\left(\left(0.5 \times CONC_{drw,L}\right) + \left(0.5 \times CONC_{drw,R}\right)\right) \times IH_{drw}}{BW} \quad \textbf{Equation 113}$$

Explanation of symbols

$CONC_{drw,L}$	Local concentration in drinking water	[mg.L^{-1}]	Equation 110
$CONC_{drw,R}$	Regional concentration in drinking water	[mg.L^{-1}]	Equation 112
IH_{drw}	Daily intake of drinking water	[L.d^{-1}]	2
BW	Bodyweight	[kg]	60
$DOSE_{drw}$	Daily dose via drinking water	[mg.kg^{-1}.d^{-1}]	

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 ≥ 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 31.

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 31 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 $f_{commodity}$ as the fraction of application that is intercepted by the commodity of interest and calculated $f_{commodity}$ as commodity surface area/crop leaf surface area. Where $f_{commodity}$ values were reported by Maclachlan and Hamilton (2010), these were used in the LET. Where no data was available, the authors assumed a default $f_{commodity}$ 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 $f_{commodity}$ was not reported by Maclachlan and Hamilton (2010). The basis for the $f_{commodity}$ values used in the LET are summarised in Table 30.

Table 30: $f_{commodity}$ values selected for treated crops in CLE LET

Crop	$f_{commodity}$	
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

Crop	$f_{commodity}$	
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 $f_{commodity}$ values used in the calculation of oral intake of a non-volatile co-formulant via treated crops, are reported in Table 31.

Table 31: 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)	$f_{commodity}$
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
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 114.

$$CONC_{crop,i} = \left(\frac{AR \times Napp}{CROP_{yield,i}}\right) \times f_{commodity,i}$$

Equation 114

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

Explanation of symbols

AR	Application rate for co-formulant	[g.ha^{-1}]	User input
Napp	Number of application events	[-]	User input
$CROP_{yield,i}$	Crop yield	[t.ha^{-1}]	Table 31
$f_{commodity,i}$	Commodity fraction of crop	[-]	Table 31
$CONC_{crop,i}$	Concentration in harvested crop	[mg.kg^{-1}]	

Daily intake of each treated crop is calculated using Equation 115.

$$INTAKE_{crop,i} = \frac{CROP_{intake,i} \times CONC_{crop,i}}{BW}$$ **Equation 115**

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

Explanation of symbols

$CROP_{intake,i}$	Daily crop consumption	[kg.day^{-1}]	Table 31
$CONC_{crop,i}$	Concentration in harvested crop	[mg.kg^{-1}]	Equation 114
BW	Bodyweight	[kg]	60
$INTAKE_{crop,i}$	Daily intake per crop	[mg.kg^{-1}.day^{-1}]	

If application is a spray and vapour pressure at 25 °C is ≥ 0.01 Pa:

$$DOSE_{crop} = 0$$ **Equation 116**

Explanation of symbols

$DOSE_{crop}$	Daily dose via crops	[mg.kg^{-1}.d^{-1}]	

For all other application types and for sprays where vapour pressure at 25 °C is < 0.01 Pa:

$$DOSE_{crop} = \sum INTAKE_{crop,i}$$ **Equation 117**

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

Explanation of symbols

$INTAKE_{crop,i}$	Daily intake from crops of i	[mg.kg^{-1}.day^{-1}]	Equation 115
$DOSE_{crop}$	Daily dose via treated crops	[mg.kg^{-1}.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).

$$C_{crop,fodder} = \frac{(AR \times Napp) \times f_{int} \times f_{commodity\ fodder}}{Y_{commodity}}$$ **Equation 118**

Explanation of symbols

AR	Application rate for co-formulant	[g.ha^{-1}]	User input

Napp	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	[$t.ha^{-1}$]	14.7
$C_{crop,fodder}$	Concentration in fodder crops	[$mg.kg_{wwt}^{-1}$]	

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 119.

$$IC_{grass} = ICdwt_{grass} \times CONV_{grass}$$ **Equation 119**

Explanation of symbols

$ICdwt_{grass}$	Daily intake of grass (dry weight)	[$kg_{dwt}.day^{-1}$]	16.9
$CONV_{grass}$	Conversion dry to wet weight grass	[$kg_{wwt}.kg_{dwt}^{-1}$]	4
IC_{grass}	Daily intake of grass (wet weight)	[$kg_{wwt}.day^{-1}$]	

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 120).

$$C_{soil} = Clocal_{soil,humans\ via\ env} + PEC_{regional\ agr.soil}$$ **Equation 120**

Explanation of symbols

$Clocal_{soil,humans\ via\ env}$	Local concentration in soil (wet weight) used in humans via the environment calculations (180d time weighted average)	[$mg.kg_{wwt}^{-1}$]	Equation 41
$PEC_{regional\ agr.soil}$	Regional concentration in agricultural soil	[$mg.kg_{wwt}^{-1}$]	Input (calculated outside LET) otherwise assumed to be 0
C_{soil}	Concentration in soil	[$mg.kg_{wwt}^{-1}$]	

The daily intake of soil by cattle is calculated using Equation 121.

$$IC_{soil} = ICdwt_{soil} \times CONV_{soil}$$ **Equation 121**

Explanation of symbols

$ICdwt_{soil}$	Daily intake of soil (dry weight)	[$kg_{dwt}.day^{-1}$]	0.41
$CONV_{soil}$	Conversion factor for soil concentration wet-dry weight soil	[$kg_{wwt}.kg_{dwt}^{-1}$]	Equation 97
IC_{soil}	Daily intake of soil (wet weight)	[$kg_{wwt}.day^{-1}$]	

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.

$$C_{air} = C_{daily,air}$$ **Equation 122**

Explanation of symbols

$C_{daily,air}$	Daily concentration in air	[mg.m^{-3}]	Equation 104
C_{air}	Concentration in air	[mg.m^{-3}]	

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 123. 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.

$$C_{drw} = \max\left(PEClocal_{gw\_dw}, PEClocal_{sw\_dw}\right)$$ **Equation 123**

Explanation of symbols

$PEClocal_{gw\_dw}$	Predicted environmental concentration in soil porewater (drinking water)	[mg.L^{-1}]	Equation 107
$PEClocal_{sw\_dw}$	Predicted environmental concentration in surface water (drinking water)	[mg.L^{-1}]	Equation 108
C_{drw}	Concentration in drinking water	[mg.L^{-1}]	

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 32.

Table 32: Bioaccumulation factor for milk (EU TGD (2003b), EUSES 2.1)

	Log Kow		
	< 3	≥ 3 - ≤ 6.5	> 6.5
BAF_{milk}	$10^{-8.1+3}$	$10^{-8.1+\log Kow}$	$10^{-8.1+6.5}$

$$C_{milk} = BAF_{milk} \times \left(IC_{grass} \times C_{crop,fodder} + IC_{soil} \times C_{soil} + IC_{air} \times C_{air} + IC_{drw} \times C_{drw}\right)$$ **Equation 124**

Explanation of symbols

BAF_{milk}	Bioaccumulation factor for milk	[day.kg$_{milk}^{-1}$]	Table 32
IC_{grass}	Daily intake of grass (wet weight)	[kg$_{wwt}$.day^{-1}]	Equation 119
$C_{crop,\ fodder}$	Concentration in fodder crops	[mg.kg$_{wwt}^{-1}$]	Equation 118
IC_{soil}	Daily intake of soil (wet weight)	[kg$_{wwt}$.day^{-1}]	Equation 121
C_{soil}	Concentration in soil	[mg.kg$_{wwt}^{-1}$]	Equation 120

IC_{air}	Daily inhalation rate of cattle	[$m^3.day^{-1}$]	122
C_{air}	Concentration in air	[$mg.m^{-3}$]	Equation 122
IC_{drw}	Daily intake of drinking water for cattle	[$L.day^{-1}$]	55
C_{drw}	Concentration in drinking water	[$mg.L^{-1}$]	Equation 123
C_{milk}	Concentration in milk	[$mg.kg_{milk}^{-1}$]	

The daily dose through intake of dairy products is then calculated using Equation 125.

$$DOSE_{dairy} = \frac{C_{milk} \times IH_{milk}}{BW}$$ **Equation 125**

Explanation of symbols

C_{milk}	Concentration in milk	[$mg.kg_{milk}^{-1}$]	Equation 124
IH_{milk}	Daily intake of dairy products	[$kg_{milk}.d^{-1}$]	0.561
BW	Bodyweight	[kg]	60
$DOSE_{dairy}$	Daily dose via dairy products	[$mg.kg^{-1}.d^{-1}$]	

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 33.

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

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

$$C_{meat} = BAF_{meat} \times \left(IC_{grass} \times C_{crop,fodder} + IC_{soil} \times C_{soil} + IC_{air} \times C_{air} + IC_{drw} \times C_{drw}\right)$$ **Equation 126**

Explanation of symbols

BAF_{meat}	Bioaccumulation factor for meat	[$day.kg_{meat}^{-1}$]	Table 33
IC_{grass}	Daily intake of grass (wet weight)	[$kg_{wwt}.day^{-1}$]	Equation 119
$C_{crop,fodder}$	Concentration in fodder crops	[$mg.kg_{wwt}^{-1}$]	Equation 118
IC_{soil}	Daily intake of soil (wet weight)	[$kg_{wwt}.day^{-1}$]	Equation 121
C_{soil}	Concentration in soil	[$mg.kg_{wwt}^{-1}$]	Equation 120
IC_{air}	Daily inhalation rate of cattle	[$m^3.day^{-1}$]	122
C_{air}	Concentration in air	[$mg.m^{-3}$]	Equation 122
IC_{drw}	Daily intake of drinking water for cattle	[$L.day^{-1}$]	55
C_{drw}	Concentration in drinking water	[$mg.L^{-1}$]	Equation 123

C_{meat}	Concentration in meat	[mg.kg$_{meat}^{-1}$]	

The daily dose through intake of meat products is then calculated using Equation 127.

$$DOSE_{meat} = \frac{C_{meat} \times IH_{meat}}{BW}$$ **Equation 127**

Explanation of symbols

C_{meat}	Concentration in meat	[mg.kg$_{meat}^{-1}$]	Equation 126
IH_{meat}	Daily intake of meat	[kg$_{meat}$.d^{-1}]	0.301
BW	Bodyweight	[kg]	60
$DOSE_{meat}$	Daily dose via meat	[mg.kg^{-1}.d^{-1}]	

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. As a screening assessment, no dilution factor is included 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 Kow using the approach discussed for secondary poisoning (Section 3.6.4). The units are converted for the humans via environment assessment using Equation 128.

$$BCF_{fish} = \frac{BCF_{fish}}{1000}$$ **Equation 128**

Explanation of symbols

BCF_{fish}	Bioconcentration factor for fish	[L.kg$_{wet\ fish}^{-1}$]	Measured or estimated from log K_{ow} (Equation 85 and Equation 86)
BCF_{fish}	Bioconcentration factor for fish	[m^3.kg$_{wwt}^{-1}$]	

$$C_{water} = \frac{Clocal_{sw,HvE,fish} + PECregional_{sw}}{1000000}$$ **Equation 129**

Explanation of symbols

$Clocal_{sw,HvE,fish}$	21 day time weighted average in surface water	[µg.L^{-1}]	Equation 83
$PECregional_{sw}$	Regional predicted environmental concentration in surface water	[µg.L^{-1}]	Input (calculated outside LET) otherwise assumed to be 0
C_{water}	Concentration in surface water	[kg.m^3]	

The concentration in fish consumed by humans is estimated according to Equation 130.

$$C_{fish} = BCF_{fish} \times C_{water} \times 1000000$$ **Equation 130**

Explanation of symbols

BCF_{fish}	Bioconcentration factor for fish	[$m^3.kg_{wwt}^{-1}$]	Equation 128
C_{water}	Concentration in surface water	[$kg.m^{-3}$]	Equation 129
C_{fish}	Concentration in wet fish	[$mg.kg_{wwt}^{-1}$]	

The daily dose through intake of fish is calculated using Equation 131.

$$DOSE_{fish} = \frac{C_{fish} \times IH_{fish}}{BW}$$ **Equation 131**

Explanation of symbols

C_{fish}	Concentration in fish	[$mg.kg_{wwt}^{-1}$]	Equation 130
IH_{fish}	Daily intake of fish	[$kg_{wwt}.d^{-1}$]	0.115
BW	Bodyweight	[kg]	60
$DOSE_{fish}$	Daily dose via fish	[$mg.kg^{-1}.d^{-1}$]	

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 132 to Equation 136. Where regional concentrations are not available, the $PEC_{compartment}$ = $Clocal_{compartment}$.

PEC Fresh Water (Pelagic)

$$PECsw = Clocal_{sw\,max} + PECregional_{sw}$$ **Equation 132**

Explanation of symbols

$PECregional_{sw}$	Freshwater concentration at the regional scale	[µg.L^{-1}]	Calculated outside the LET
$Clocal_{sw\ max}$	Maximum local freshwater concentration	[µg.L^{-1}]	Equation 74
PECsw	Predicted environmental concentrations in freshwater	[µg.L^{-1}]	

PEC Fresh Water (Sediment)

$$PECsed = Clocal_{sed\ max} + PECregional_{sed}$$ **Equation 133**

Explanation of symbols

$PECregional_{sed}$	Freshwater sediment concentration at the regional scale (dry weight)	[µg.kg $_{dwt}^{-1}$]	Calculated outside the LET
$Clocal_{sed\ max}$	Maximum local freshwater sediment concentration (dry weight)	[µg.kg $_{dwt}^{-1}$]	Equation 75
PECsed	Predicted environmental concentrations in freshwater sediment (dry weight)	[µg.kg $_{dwt}^{-1}$]	

PEC Marine Water (Pelagic)

$$PECmarine\ water = Clocal_{marine\ water} + PECregional_{marine\ water}$$ **Equation 134**

Explanation of symbols

$PECregional_{marine\ water}$	Marine water concentration at the regional scale	[µg.L^{-1}]	Calculated outside the LET
$Clocal_{marine\ water}$	Local marine water concentration	[µg.L^{-1}]	Equation 76
PECmarine water	Predicted environmental concentration in marine water	[µg.L^{-1}]	

PEC Marine Water (Sediment)

$$PECmarine\ sediment = Clocal_{marine\ sediment} + PECregional_{marine\ sediment}$$ **Equation 135**

Explanation of symbols

$PECregional_{marine\ sediment}$	Marine sediment concentration at the regional scale (dry weight)	[µg.kg $_{dwt}^{-1}$]	Calculated outside the LET
$Clocal_{marine\ sediment}$	Local marine sediment concentration (dry weight)	[µg.kg $_{dwt}^{-1}$]	Equation 77
PECmarine sediment	Predicted environmental concentration in marine sediment (dry weight)	[µg.kg $_{dwt}^{-1}$]	

PEC Soil

$$PECsoil = Clocal_{soil} + PECregional_{agric.soil}$$ **Equation 136**

Explanation of symbols

$PECregional_{agric.soil}$	Agricultural soil concentration at the regional scale (dry weight)	[µg.kg $_{dwt}^{-1}$]	Calculated outside the LET
$Clocal_{soil}$	Local soil concentration (30 day TWA) (dry weight)	[µg.kg $_{dwt}^{-1}$]	Equation 39
PECsoil	Predicted environmental concentration in soil (dry weight)	[µg.kg $_{dwt}^{-1}$]	

3.6.6.2 RCR calculations

The risk characterisation ratios (RCRs) for each relevant environmental compartment are calculated using Equation 137.

$$RCR_{compartment} = \frac{PEC_{compartment}}{PNEC_{compartment}}$$ **Equation 137**

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 138.

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

$$RCR_{compartment} = \frac{PEC_{compartment}}{PNEC_{compartment}} \times 10$$ **Equation 138**

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 139.

$$RCR_{inhalation} = \frac{DOSE_{air}}{DNEL_{inhalation}}$$ **Equation 139**

Explanation of symbols

$DOSE_{air}$	Daily dose via inhalation	[mg.m^{-3}] [mg.kg^{-1}.d^{-1}]	Equation 105/ Equation 106
$DNEL_{inhalation}$	General population, systemic effects, long term inhalation DNEL	[mg.m^{-3}] [mg.kg^{-1}.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 140.

$$RCR_{oral,i} = \frac{DOSE_i}{DNEL_{oral}}$$ **Equation 140**

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

Explanation of symbols

$DOSE_{oral,i}$	Daily dose via oral route i	[mg.kg^{-1}.d^{-1}]	Equation 111 or Equation 113, Equation 116 or Equation 117, Equation 125, Equation 127, Equation 131
$DNEL_{oral}$	General population, systemic effects, long term oral DNEL	[mg.kg^{-1}.d^{-1}]	User input
RCR_i	RCR oral via route i	[-]	

The overall RCR for humans via the environment is calculated using Equation 141.

$$RCR_{total} = \left(\sum RCR_{oral,i}\right) + RCR_{inhalation}$$ **Equation 141**

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

Explanation of symbols

$RCR_{oral,i}$	RCR oral via route i	[-]	Equation 140
$RCR_{inhalation}$	RCR inhalation	[-]	Equation 139
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^{-1}. 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 142 (initially AR = 1 kg.ha^{-1}) 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.

$$SafeDose_{compartment} = \left(\frac{AR}{RCR_{compartment} - \frac{PEC\ Reg_{compartment}}{PNEC_{compartment}}}\right) \times \left(TargetRCR - \frac{PEC\ Reg_{compartment}}{PNEC_{compartment}}\right) \quad \textbf{Equation 142}$$

Explanation of symbols

$PNEC_{compartment}$	Predicted no effect concentration for the environmental compartment		
AR	Application rate for co-formulant	[kg.ha^{-1}]	User input
$RCR_{compartment}$	RCR for the environmental compartment, using the original application rate (AR)	[-]	
Target RCR	RCR target	[-]	Default = 0.90
$PEC\ Reg_{compartment}$	Predicted environmental concentration from the background (PECregional) for the environmental compartment		
$SafeDose_{compartment}$	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 143).

$$PEC\ Reg_{compartment} = PECregional_{compartment} \quad \textbf{Equation 143}$$

For aquatic and terrestrial predators, the safe dose is calculated using Equation 144 to Equation 146. Again, the maximum dose acceptable for the most sensitive environmental compartment for the substance assessed is reported as the estimated safe dose.

$$SafeDose_{compartment} = \left(\frac{AR}{RCR_{local\ concentration}}\right) \times TargetRCR_{local\ concentration} \quad \textbf{Equation 144}$$

Where:

$$RCR_{local\ concentration} = \left(F_{local\ diet} \times \frac{\text{PEC Local}_{\text{compartment}}}{\text{PNEC}_{\text{compartment}}}\right) - \left(F_{local\ diet} \times \frac{PEC\ \text{Background}_{compartment}}{PNEC_{compartment}}\right) \quad \textbf{Equation 145}$$

$$TargetRCR_{local\ concentration} = TargetRCR - \left(F_{\text{local diet}} \times \frac{PEC\ background_{compartment}}{PNEC_{compartment}}\right) - \left(F_{\text{regional diet}} \times \frac{PEC\ R \rightleftarrows eg_{compartment}}{PNEC_{compartment}}\right) \quad \textbf{Equation 146}$$

Explanation of symbols

AR	Application rate for co-formulant	[kg.ha^{-1}]	User input
$RCR_{local\ concentration}$	Local concentration RCR	[-]	Equation 145
$TargetRCR_{local\ concentration}$	Local concentration RCR target	[-]	Equation 146
$F_{local\ diet}$	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 (PECregional) 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
$PEC\ Reg_{compartment}$	Predicted environmental concentration at the regional scale (PECregional) 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 147 to Equation 157. 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:

$$PEC\ Background_{compartment} = PECregional_{oral,predator} \quad \textbf{Equation 147}$$

$$PEC\ Reg_{compartment} = PECregional_{oral,predator} \quad \textbf{Equation 148}$$

$$PECregional_{oral,predator} = PECregional_{sw\ or\ mw(dissolved)} \times BCF_{fish} \times BMF_1 \quad \textbf{Equation 149}$$

Marine top predator:

$$PEC\ Background_{compartment} = PECregional_{oral,toppredator} \quad \textbf{Equation 150}$$

$$PEC\ Reg_{compartment} = PECregional_{oral,toppredator} \quad \textbf{Equation 151}$$

$$PECregional_{oral,toppredator} = PECregional_{mw\ (dissolved)} \times BCF_{fish} \times BMF_1 \times BMF_2$$ **Equation 152**

Terrestrial Predator:

$$PEC\ Background_{compartment} = PECregional_{oral,predator}$$ **Equation 153**

For the calculation of background exposure of terrestrial predators at the local scale (Equation 153), the $Regional_{porewater}$ is calculated directly from the regional PEC in agricultural soil (Equation 154).

$$Regional_{porewater} = \left(\frac{PEC_{regional\ agric.\ soil} \times RHO_{soil}}{Ksoil - water \times 1000}\right)$$ **Equation 154**

$$PEC\ Reg_{compartment} = PECregional_{oral,predator}$$ **Equation 155**

For the calculation of exposure of terrestrial predators at the regional scale (Equation 155) the $Regional_{porewater}$ is taken directly as the regional PEC in porewater of agricultural soil (Equation 156).

$$Regional_{porewater} = PECregional_{agric\ soil\ porewater}$$ **Equation 156**

$$PEC_{oralpredator} = \frac{BCF_{earthworm} \times Regional_{porewater} + Regional_{agric.soil} \times F_{gut} \times CONV_{soil}}{1 + F_{gut} \times CONV_{soil}}$$ **Equation 157**

For humans via the environment where General Population DNELs for both inhalation and oral routes are available, the safe dose is calculated using Equation 158.

$$SafeDose = \left(\frac{(TargetRCR - \sum RegionalRCR_i)}{\sum LocalRCR_i}\right) \times AR$$ **Equation 158**

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

Explanation of symbols

Target RCR	RCR target	[-]	Default = 0.90
RegionalRCR$_i$	Regional RCR via route i	[-]	Equation 161 or Equation 162, Equation 163, Equation 164, Equation 166, Equation 168
LocalRCR$_i$	Local RCR via route i	[-]	Equation 169 or Equation 170, Equation 171, Equation 172, Equation 173, Equation 176, Equation 178
AR	Application rate for co-formulant	[kg.ha^{-1}]	User Input
SafeDose	Application rate at target RCR	[kg.ha^{-1}]	

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 159Equation 137.

$$SafeDose = \left(\frac{(TargetRCR - RegionalRCR_{inhalation})}{LocalRCR_{inhalation}}\right) \times AR$$ **Equation 159**

Explanation of symbols

Target RCR	RCR target	[-]	Default = 0.90
$RegionalRCR_{inhalation}$	Regional RCR via inhalation	[-]	Equation 161 or Equation 162
$LocalRCR_{inhalation}$	Local RCR via inhalation	[-]	Equation 170
AR	Application rate for co-formulant	[kg.ha^{-1}]	User Input
SafeDose	Application rate at target RCR	[kg.ha^{-1}]	

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 160.

$$SafeDose = \left(\frac{(TargetRCR - \sum RegionalRCR_i)}{\sum LocalRCR_i}\right) \times AR$$ **Equation 160**

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

Explanation of symbols

Target RCR	RCR target	[-]	Default = 0.90
$RegionalRCR_i$	Regional RCR via route i	[-]	Equation 163, Equation 164, Equation 166, Equation 168
$LocalRCR_i$	Local RCR via route i	[-]	Equation 171, Equation 172, Equation 173, Equation 176, Equation 178
AR	Application rate for co-formulant	[kg.ha^{-1}]	User Input
SafeDose	Application rate at target RCR	[kg.ha^{-1}]	

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^3, the regional $RCR_{inhalation}$ is calculated as:

$$Regional\ RCR_{inhalation} = \frac{PECregional_{air}}{DNEL_{inhalation}}$$ **Equation 161**

Explanation of symbols

$PECregional_{air}$	Regional PEC in air	[mg.m^{-3}]	Input (calculated

			outside LET)
$DNEL_{inhalation}$	General population, systemic effects, long term inhalation DNEL	[mg.m^{-3}]	User input
Regional $RCR_{inhalation}$	Regional RCR for inhalation	[-]	

If the General Population DNEL for inhalation is in mg/kg bw/day, the regional $RCR_{inhalation}$ is calculated:

$$Regional\ RCR_{inhalation} = \frac{\left(\frac{PECregional_{air} \times F_{resp} \times IH_{air}}{BW} \times \frac{BIO_{inh}}{BIO_{oral}}\right)}{DNEL_{inhalation}} \qquad \textbf{Equation 162}$$

Explanation of symbols

$PECregional_{air}$	Regional PEC in air	[mg.m^{-3}]	Input (calculated outside LET)
F_{resp}	Respirable fraction of inhaled substance	[-]	1
IH_{air}	Daily intake of air	[m^3.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.kg^{-1}.d^{-1}]	User input
Regional $RCR_{inhalation}$	Regional RCR for inhalation	[-]	

The $RegionalRCR_i$ includes regional RCRs for drinking water, treated crops, milk, meat and fish. The Regional RCR for drinking water is calculated as:

$$RegionalRCR_{drw} = 0.5 \times \left(\frac{\frac{CONC_{drw,R} \times IH_{drw}}{BW}}{DNEL_{oral}}\right) + 0.5 \times \left(\frac{\frac{CONC_{drw,R} \times IH_{drw}}{BW}}{DNEL_{oral}}\right) \qquad \textbf{Equation 163}$$

Explanation of symbols

$CONC_{drw,R}$	Regional concentration in drinking water	[mg.L^{-1}]	Equation 112
IH_{drw}	Daily intake of drinking water	[L.d^{-1}]	2
BW	Bodyweight	[kg]	60
$DNEL_{oral}$	General population, systemic effects, long term oral DNEL	[mg.kg^{-1}.d^{-1}]	User input
Regional RCR_{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:

$$Regional\ RCR_{fish} = \frac{\left(\frac{\left(BCF_{fish} \times PECregional_{sw} \times 1000000\right) \times IH_{fish}}{BW}\right)}{DNEL_{oral}}$$ **Equation 164**

Explanation of symbols

BCF_{fish}	Bioconcentration factor for fish	[$m^3.kg_{wwt}^{-1}$]	Equation 128
$PECregional_{sw}$	Regional predicted environmental concentration in surface water	[$kg.m^3$]	Input (calculated outside LET)
IH_{fish}	Daily intake of fish	[$kg_{wwt}.d^{-1}$]	0.115
BW	Bodyweight	[kg]	60
$DNEL_{oral}$	General population, systemic effects, long term oral DNEL	[$mg.kg^{-1}.d^{-1}$]	User input
$Regional\ RCR_{fish}$	Regional RCR for fish intake	[-]	

The Regional PEC for intake via dairy products is calculated using Equation 165 where regional intake from treated crops is zero and the Regional RCR for intake via dairy products is calculated using Equation 166.

$$Regional\ PEC_{milk} = BAF_{milk} \times \left(IC_{soil} \times PECregional_{soil} + IH_{air} \times PECregional_{air} + IC_{drw} \times CONC_{drw,R}\right)$$ **Equation 165**

Explanation of symbols

BAF_{milk}	Bioaccumulation factor for milk	[$day.kg_{milk}^{-1}$]	Table 32
IC_{soil}	Daily intake of soil (wet weight)	[$kg_{wwt}.day^{-1}$]	Equation 121
$PECregional_{soil}$	Regional PEC in soil	[$mg.kg_{wwt}^{-1}$]	Input (calculated outside LET)
IH_{air}	Daily inhalation rate of cattle	[$m^3.day^{-1}$]	122
$PECregional_{air}$	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 112
$Regional\ PEC_{milk}$	Regional concentration in milk	[$mg.kg_{milk}^{-1}$]	

$$Regional\ RCR_{dairy} = \frac{\left(\frac{Regional\ PEC_{milk} \times IH_{milk}}{BW}\right)}{DNEL_{oral}}$$ **Equation 166**

Explanation of symbols

$Regional\ PEC_{milk}$	Regional concentration in milk	[$mg.kg_{milk}^{-1}$]	Equation 165
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 167 where regional intake from treated crops is zero and the Regional RCR for intake via meat is calculated using Equation 168.

$$Regional\ PEC_{meat} = BAF_{meat} \times \left(IC_{soil} \times PECregional_{soil} + IH_{air} \times PECregional_{air} + IC_{drw} \times CONC_{drw,R}\right)$$ **Equation 167**

Explanation of symbols

BAF_{meat}	Bioaccumulation factor for meat	[day.kg_{milk}^{-1}]	Table 33
IC_{soil}	Daily intake of soil (wet weight)	[kg_{wwt}.day^{-1}]	Equation 121
$PECregional_{soil}$	Regional PEC in soil	[mg.kg_{wwt}^{-1}]	Input (calculated outside LET)
IH_{air}	Daily inhalation rate of cattle	[m^3.day^{-1}]	122
$PECregional_{air}$	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 112
Regional PEC_{meat}	Regional concentration in meat	[mg.kg_{meat}^{-1}]	

$$Regional\ RCR_{meat} = \frac{\left(\frac{Regional\ PEC_{meat} \times IH_{meat}}{BW}\right)}{DNEL_{oral}}$$ **Equation 168**

Explanation of symbols

Regional PEC_{meat}	Regional concentration in meat	[mg.kg_{meat}^{-1}]	Equation 167
IH_{meat}	Daily intake of meat	[kg_{meat}.d^{-1}]	0.301
BW	Bodyweight	[kg]	60
$DNEL_{oral}$	General population, systemic effects, long term oral DNEL	[mg.kg^{-1}.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:

$$Local\ RCR_{inhalation} = \frac{C_{daily,air} - PECregional_{air}}{DNEL_{inhalation}}$$ **Equation 169**

Explanation of symbols

$C_{daily,air}$	Daily concentration in air	[mg.m^{-3}]	Equation 104

$PECregional_{air}$	Regional PEC in air	[mg.m^{-3}]	Input (calculated outside LET)
$DNEL_{inhalation}$	General population, systemic effects, long term inhalation DNEL	[mg.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:

$$Local\ RCR_{inhalation} = \frac{\left(\frac{\left(C_{daily,air} - PECregional_{air}\right) \times F_{resp} \times IH_{air}}{BW} \times \frac{BIO_{inh}}{BIO_{oral}}\right)}{DNEL_{inhalation}} \qquad \textbf{Equation 170}$$

Explanation of symbols

$C_{daily,air}$	Daily concentration in air	[mg.m^{-3}]	Equation 104
$PECregional_{air}$	Regional PEC in air	[mg.m^{-3}]	Input (calculated outside LET)
F_{resp}	Respirable fraction of inhaled substance	[-]	1
IH_{air}	Daily intake of air	[m^3.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.kg^{-1}.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:

$$LocalRCR_{drw} = 0.5 \times \left(\frac{\frac{CONC_{drw,L} \times IH_{drw}}{BW}}{DNEL_{oral}}\right) - 0.5 \times \left(\frac{\frac{CONC_{drw,R} \times IH_{drw}}{BW}}{DNEL_{oral}}\right) \qquad \textbf{Equation 171}$$

Explanation of symbols

$CONC_{drw,\ L}$	Local concentration in drinking water	[mg.L^{-1}]	Equation 110
$CONC_{drw,R}$	Regional concentration in drinking water	[mg.L^{-1}]	Equation 112
IH_{drw}	Daily intake of drinking water	[L.d^{-1}]	2
BW	Bodyweight	[kg]	60
$DNEL_{oral}$	General population, systemic effects, long term oral DNEL	[mg.kg^{-1}.d^{-1}]	User input
$Local\ RCR_{drw}$	Local RCR for drinking water	[-]	

As there is no regional contribution to treated crops, the Local RCR for treated crops is:

$$Local\ RCR_{crop} = \frac{DOSE_{crop}}{DNEL_{oral}}$$ **Equation 172**

Explanation of symbols

$DOSE_{crop}$	Daily dose via crops	[mg.kg^{-1}.bw^{-1}]	Equation 117
$DNEL_{oral}$	General population, systemic effects, long term oral DNEL	[mg.kg^{-1}.d^{-1}]	User input
$Local\ RCR_{crop}$	Local RCR for crops	[-]	

The Local RCR for intake via fish is calculated as:

$$Local\ RCR_{fish} = \frac{\left(\frac{\left(BCF_{fish} \times Clocal_{sw,HvE,fish} \times 1000000\right) \times IH_{fish}}{BW}\right)}{DNEL_{oral}}$$ **Equation 173**

Explanation of symbols

BCF_{fish}	Bioconcentration factor for fish	[m^3.kg$_{wwt}^{-1}$]	Equation 128
$Clocal_{sw,HvE,fish}$	21 day time weighted average in surface water	[µg.L^{-1}]	Equation 83
IH_{fish}	Daily intake of fish	[kg$_{wwt}$.d^{-1}]	0.115
BW	Bodyweight	[kg]	60
$DNEL_{oral}$	General population, systemic effects, long term oral DNEL	[mg.kg^{-1}.d^{-1}]	User input
$Local\ RCR_{fish}$	Local RCR for fish intake	[-]	

The Local PEC for intake via dairy products is calculated using Equation 174 and the Local RCR for intake via dairy products is calculated using Equation 176.

$$\begin{aligned} Local\ PEC_{milk} = {} & BAF_{milk} \\ & \times \left(IC_{grass} \times C_{crop,fodder} + IC_{soil} \times TWAC_{soil(180d)}\right. \\ & \left. + IH_{air} \times \left(C_{field,air,24\,h} \times 1000000\right) + IC_{drw} \times Local_{drw}\right) \end{aligned}$$ **Equation 174**

Explanation of symbols

BAF_{milk}	Bioaccumulation factor for milk	[day.kg$_{milk}^{-1}$]	Table 32
IC_{grass}	Daily intake of grass (wet weight)	[kg$_{wwt}$.day^{-1}]	Equation 119
$C_{crop,fodder}$	Concentration in fodder crops	[mg.kg$_{wwt}^{-1}$]	Equation 118
IC_{soil}	Daily intake of soil (wet weight)	[kg$_{wwt}$.day^{-1}]	Equation 121
$TWAC_{soil(180d)}$	Local concentration in soil (wet weight) as a 180d time weighted average	[mg.kg$_{wwt}^{-1}$]	Equation 41
IH_{air}	Daily inhalation rate of cattle	[m^3.day^{-1}]	122
$C_{field,air,24\,h}$	24 hour averaged concentration at 10 metres downwind of field	[kg.m^{-3}]	Equation 103
IC_{drw}	Daily intake of drinking water for cattle	[L.day^{-1}]	55

$Local_{drw}$	Local concentration in drinking water	[mg.L^{-1}]	Equation 175
Local PEC$_{milk}$	Local concentration in milk	[mg.kg$_{milk}^{-1}$]	

$$If\ CONC_{drw,L} = Groundwater, \text{then:}$$
$$Local_{drw} = PEClocal_{gw\_dw} - PECregional_{porewater}$$
$$If\ CONC_{drw,L} = Surfacewater, \text{then:}$$
$$Local_{drw} = PEClocal_{sw\_dw}$$

Equation 175

Explanation of symbols

$CONC_{drw,\ L}$	Local concentration in drinking water	[mg.L^{-1}]	Equation 110
$PEClocal_{gw\_dw}$	Predicted environmental concentration in soil porewater (drinking water)	[mg.L^{-1}]	Equation 107
$PECregional_{porewater}$	Regional PEC in porewater	[mg.L^{-1}]	Input (calculated outside LET)
$PEClocal_{sw\_dw}$	Predicted environmental concentration in surface water (drinking water)	[mg.L^{-1}]	Equation 108
$Local_{drw}$	Local concentration in drinking water	[mg.L^{-1}]	

$$Local\ RCR_{dairy} = \frac{\left(\frac{Local\ PEC_{milk} \times IH_{milk}}{BW}\right)}{DNEL_{oral}}$$

Equation 176

Explanation of symbols

Local PEC$_{milk}$	Local concentration in milk	[mg.kg$_{milk}^{-1}$]	Equation 174
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
Local RCR$_{dairy}$	Local RCR for dairy products	[-]	

The Local PEC for intake via meat is calculated using Equation 177 and the Local RCR for intake via meat is calculated using Equation 178.

$$Local\ PEC_{meat} = BAF_{meat} \times \left(IC_{grass} \times C_{crop} + IC_{soil} \times TWAC_{soil(180d)} + IH_{air} \times (C_{field,air,24\,h} \times 1000000) + IC_{drw} \times Local_{drw}\right)$$

Equation 177

Explanation of symbols

BAF_{meat}	Bioaccumulation factor for meat	[day.kg$_{milk}^{-1}$]	Table 33
IC_{grass}	Daily intake of grass (wet weight)	[kg$_{wwt}$.day^{-1}]	Equation 119
C_{crop}	Concentration in fodder crops	[mg.kg$_{wwt}^{-1}$]	Equation 118
IC_{soil}	Daily intake of soil (wet weight)	[kg$_{wwt}$.day^{-1}]	Equation 121

$TWAC_{soil(180d)}$	Local concentration in soil (wet weight) as a 180d time weighted average	[$mg.kg_{wwt}^{-1}$]	Equation 41
IH_{air}	Daily inhalation rate of cattle	[$m^3.day^{-1}$]	122
$C_{field,air,24\ h}$	24 hour averaged concentration at 10 metres downwind of field	[$kg.m^{-3}$]	Equation 103
IC_{drw}	Daily intake of drinking water for cattle	[$L.day^{-1}$]	55
$Local_{drw}$	Local concentration in drinking water	[$mg.L^{-1}$]	Equation 175
$Local\ PEC_{meat}$	Local concentration in meat	[$mg.kg_{meat}^{-1}$]	

$$Local\ RCR_{meat} = \frac{\left(\frac{Local\ PEC_{meat} \times IH_{meat}}{BW}\right)}{DNEL_{oral}}$$ **Equation 178**

Explanation of symbols

$Local\ PEC_{meat}$	Local concentration in meat	[$mg.kg_{meat}^{-1}$]	Equation 177
IH_{meat}	Daily intake of meat	[$kg_{meat}.d^{-1}$]	0.301
BW	Bodyweight	[kg]	60
$DNEL_{oral}$	General population, systemic effects, long term oral DNEL	[$mg.kg^{-1}.d^{-1}$]	User input
$Local\ RCR_{meat}$	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 SPECFIC 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

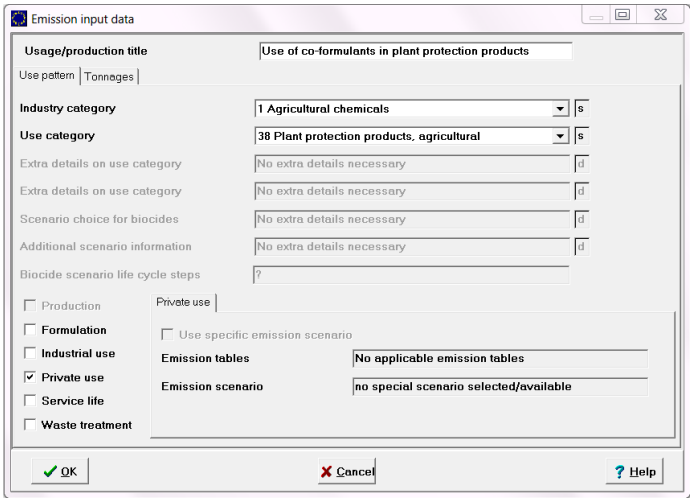
3.7.5 How to use the CLE SpERCs in EUSES

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.

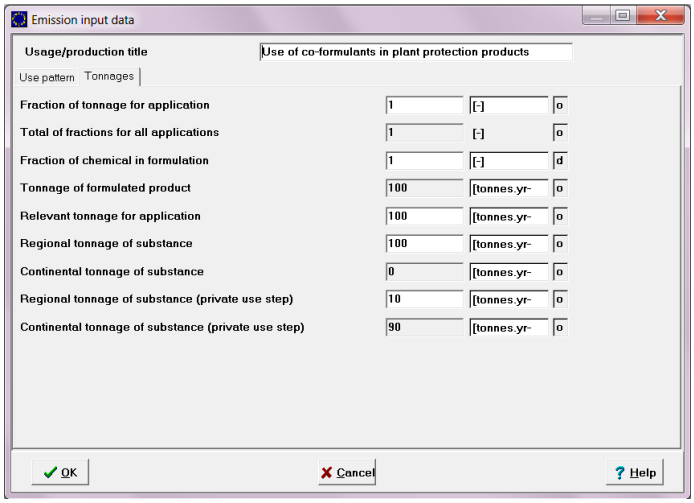
Where only a single CLE SpERC is required, it can be entered by adding a single use (e.g. "Use of co-formulants in plant protection products") in the "Release estimation" category under "Use patterns – Other life cycle steps". The emission input data should look like the following example:



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".

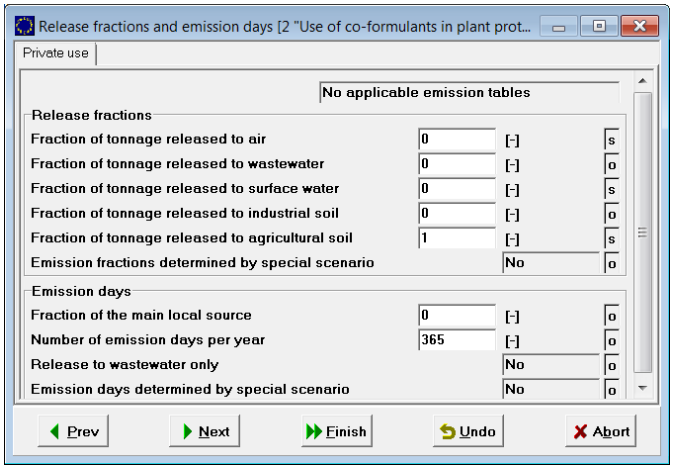
The tonnage for the use of the substance as a co-formulant needs to be appropriately defined (see 3.7.2). The fraction of the substance in the formulation is "1", since the assessment of environmental exposure will be tonnage-based and a fraction of less than 1 will not alter the final exposure estimate. 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:



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:



4 References

Brouwer DH et al.: Modeling re-entry exposure estimates: techniques and application rates, Journal: Worker exposure to agrochemicals, CRC Press, 119, p. 119-138, 2001.

Dobe C, Bonifay S, Fliege R, Krass J, Mostert V, Vosswinkel R, Wormuth M (2017), Development of REACH Generic Exposure Scenarios of substances used as coformulants in plant protection products. *Risk Analysis* 37(5), 930-942, 2017

Dobe C, Bonifay S, Krass J, McMillan C, Terry A, Wormuth M (2020), REACH Specific Environmental Release Categories for Plant Protection Product Applications. *Integrated Environmental Assessment and Management* 16(4), 472-480, 2020

ECETOC TRA Manual; Targeted Risk Assessment (User Guide for the integrated tool – TRAM, version 3); European Centre for Ecotoxicology and Toxicology of Chemicals, www.ecetoc.org

ECHA Part E (2016), Guidance on Information Requirements and Chemical Safety Assessment, Part E: Risk Characterisation, May 2016

ECHA R.10 (2008), Guidance on information requirements and chemical safety assessment, Chapter R.10: Characterisation of dose [concentration]-response for environment, May 2008

ECHA R.12 (2015), Guidance on information requirements and chemical safety assessment, Chapter R.12: Use description, December 2015.

ECHA R.14 (2016), Guidance on information requirements and chemical safety assessment, Chapter R.14: Occupational exposure estimation, August 2016

ECHA R.15 (2016), Guidance on information requirements and chemical safety assessment, Chapter R.15: Consumer exposure estimation, July 2016

ECHA R.16 (2016), Guidance on information requirements and chemical safety assessment, Chapter R.16: Environmental Exposure Estimation, February 2016

ECHA R.7a (2017), Guidance on information requirements and chemical safety assessment, Chapter R.7a: Endpoint specific guidance, July 2017

EFSA (2014), Guidance on the assessment of exposure of operators, workers, residents and bystanders in risk assessment for plant protection products. EFSA Journal 12(10), 3874

EUSES 2.1, EUSES 2.1 Background report, Chapter III Model Calculations

EU-TGD (2003), Technical Guidance Document on Risk Assessment Part 2, European Commission Joint Research Centre

EU-TGD (2003b), Technical Guidance Document on Risk Assessment Part 1, European Commission Joint Research Centre

FOCUS (2003), Appendix I Steps 1-3 in FOCUS USER Manual, FOCUS Surface water scenarios in the EU Evaluation process under 91/414/EEC, SANCO/4802/2001-rev.2 final (May 2003)

Franco A, Trapp S (2010), A multimedia activity model for ionizable compounds: Validation study with 2,4-dichlorophenoxyacetic acid, aniline, and trimethoprim. *Environ Toxicol Chem* **29**:789-799

Großkopf C, Martin S, Mielke H, Westphal D, Hamey P, Bouneb F, Rautmann D, Erdtmann-Vourliotis M, IVA Expert Committee for Operator Safety, ECPA Occupational and Bystander Exposure Expert Group, Tiramani M, Gerritsen R, Spaan S (2013), Joint development of a new Agricultural Operator Exposure Model. Bundesinstitut für Risikobewertung Project Report, 29 January 2013.

Hoernicke E et al. (1998), Hinweise in der Gebrauchsanleitung zum Schutz von Personen bei Nachfolgearbeiten in mit Pflanzenschutzmitteln behandelten Kulturen (worker re-entry), Journal: Nachrichtenbl. Deut. Pflanzenschutzd., Eugen Ulmer GmbH & Co., 50, p. 267-269,1998, (ISSN 0027-7479)

Jager T (1998): Mechanistic approach for estimating bioconcentration of organic chemicals in earthworms (Oligochaeta). *Environmental Toxicology and Chemistry* **17** (10), 2080-2090.

Krebs B et al. (2000): Uniform Principles for Safeguarding the Health of Workers Re-Entering Crop-Growing Areas after Application of Plant Protection Products, Journal: Nachrichtenbl. Deut. Pflanzenschutzd., Eugen Ulmer GmbH & Co., 52, p. 5-9, 2000.

Krieger R et al. (1992): Assessing human exposure to pesticides, Journal: Reviews of Environmental Contamination and Toxicology, Springer-Verlag, 128, p. 1-15, 1992

Lundehn JR et al. (1992). Uniform Principles for Safeguarding the Health of Applicators of Plant Protection Products (Uniform Principles for Operator Protections); *Mitteilungen aus der Biologischen Bundesanstalt für Land- und Forstwirtschaft*, Berlin-Dahlem, n° 277, 1992

Maclachlan DJ, Hamilton D. (2010): A new tool for the evaluation of crop residue trial data (day-zero plus decline). Food Additives and Contaminants 27(3), 347-364.

Mostert V, Bonifay S, Dobe C, Fliege R, Krass J, Vosswinkel R, Wormuth M (2018), REACH Worker Exposure model for co-formulants used in plant protection products, *Annals of Work Exposures and Health* 2018, 1-14

EFSA PRIMo v3: EFSA (European Food Safety Authority), Brancato A, Brocca D, Ferreira L, Greco L, Jarrah S, Leuschner R, Medina P, Miron I, Nougadere A, PedersenR, Reich H, Santos M, Stanek A, Tarazona J, Theobald A and Villamar-Bouza L, 2018. Guidance on use of EFSA Pesticide Residue Intake Model (EFSA PRIMo revision 3). EFSA Journal 2018;16(1):5147, 43 pp. https://doi.org/10.2903/j.efsa. 2018.5147

Rautmann D et al. (2001): New basic drift values in the authorization procedure for plant protection products. Mitteilungen aus der Biologischen Bundesanstalt für Land- und Forstwirtschaft, 2001, 383, 133-141.

RIVM, VROM, VWS (2002): Uniform System for the Evaluation of Substances 4.0 (USES 4.0). National Institute of Public Health and the Environment (RIVM), Ministry of Housing, Spatial Planning and the Environment (VROM), Ministry of Health, Welfare and Sport (VWS), The Netherlands, RIVM report 601450012

RIVM (2005): ConsExpo 4.0, Program Manual (RIVM Report 320104004/2005), Chapter 4.1.1, Constant rate release mode (Equation 3(a))

Sabljic and Güsten (1995): QSARs for soil sorption. In: Overview of Structure-Activity Relationships for Environmental Endpoints. Hermens JLM (ed.), Report prepared within the framework of the project "QSAR for Prediction of Fate and Effects of Chemicals in the Environment", an international project of the Environmental Technologies RTD Programme (DG XII/D-1) of the European Commission under contract number EV5V-CT92-0211.

US EPA (2012a): Occupational Pesticide Handler Unit Exposure Surrogate Reference Table, March 2012, available at http://www.epa.gov/pesticides/science/handler-exposure-table.pdf (accessed8 Jun 2012)

US EPA (2012b): 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 (accessed 8 Jun 2012))

van Hemmen JJ et al. Post-application exposure of workers to pesticides in agriculture. EUROPOEM II PROJECT FAIR3-CT96-1406. Draft Report of the Re-entry Working Group, December 2002

Veith GD, Defoe DL and Bergstedt BV (1979): Measuring and estimating the bioconcentration factor of chemicals in fish. *J. Fish Board Can.* **36**, 1040-1048.

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.

Endpoint	**Substance 1**	**Substance 2**	**Substance 3**	**Substance 4**	**Substance 5**
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
Endpoint	**Substance 6**	**Substance 7**	**Substance 8**	**Substance 9**	**Substance 10**
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.

	Maximum safe application rate (kg/ha), default assessment, one application			
	LET 3.1	**LET 4.0**	**LET 3.1**	**LET 4.0**
	Spray application	**Spray application**	**Granular application**	**Granular application**
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

Endpoint	**Test Substance 1**	**Test Substance 2**	**Test Substance 3**	**Test Substance 4**
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_{OW} (log value)	0.5	3	3.2	-0.1
Biodegradability classification	Readily biodegradable	Readily biodegradable	Not biodegradable	Readily biodegradable
QSAR for K_{OC}	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) 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 31).

Table A 7: Average crop yields (tonnage/ha) for 28 EU member states from 2011 to 2019

Crops	2011	2012	2013	2014	2015	2016	2017	2018	2019	9 year average
Pome/stone fruit (EUROSTAT crop: Apples)	19.97	17.52	19.67	21.89	22.18	19.11	16.66	23.15	20.49	**20.1**
Citrus (EUROSTAT crop: Citrus fruits)	22.14	22.03	21.10	22.97	20.84	21.02	20.63	21.84	20.40	**21.4**
Berries (EUROSTAT crop: Berries (excluding strawberries))	3.88	3.38	3.39	4.01	4.83	4.45	4.79	4.99	4.89	**4.3**
Table grapes (EUROSTAT crop: Table grapes)	9.72	10.17	10.28	9.32	9.21	9.82	9.19	10.47	10.16	**9.8**
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	**5.4**
Pulses (EUROSTAT crop: Fresh peas)	5.64	4.98	5.40	5.52	5.61	5.45	5.20	4.59	5.19	**5.3**
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	**2.9**
Root vegetables (EUROSTAT crop: Carrots)	41.78	42.33	40.77	42.67	41.18	41.99	41.56	39.99	42.20	**41.6**
Leafy vegetables (EUROSTAT crop: Lettuces)	22.89	24.01	21.84	22.11	23.77	22.66	23.38	22.95	23.09	**23.0**

Bulb vegetables (EUROSTAT crop: Onions)	32.81	32.48	31.56	33.45	31.74	30.57	29.07	27.11	29.64	**30.9**
Tomatoes (EUROSTAT crop: Tomatoes)	62.88	65.48	65.44	63.80	69.67	72.71	72.17	69.79	70.48	**68.0**
Brassica vegetables (EUROSTAT crop: Brassicas)	32.60	31.95	30.31	30.70	27.44	27.01	27.31	25.82	27.12	**28.9**
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	**14.7**

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	**2.58**	0.92	1.02	1.21	0.75	1.55	1.09	**2.58**
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	**1.91**	1.00	1.39	0.46	1.13	0.73	0.67	**1.91**
Berries (strawberries)	0.07	0.06	0.14	0.12	**0.18**	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	**0.18**
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	**1.05**	0.33	0.33	0.30	0.42	0.34	**1.05**
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	**7.23**	4.22	4.08	3.92	3.61	4.54	**7.23**
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	**0.36**	0.02	0.01	0.12	0.03	0.03	0.09	0.02	0.06	**0.36**
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	**0.54**	0.33	0.26	n.d.	0.20	**0.54**
Root vegetables (potatoes)	1.27	0.93	1.18	0.73	2.29	0.60	3.17	2.43	3.44	**5.33**	3.73	4.17	1.40	1.37	1.23	1.10	2.00	3.75	3.90	2.96	3.91	3.56	**5.33**
Leafy vegetables (lettuce)	0.09	0.54	0.14	0.18	0.09	**0.56**	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	**0.56**
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	**0.76**	0.35	0.51	0.58	0.18	0.52	**0.76**
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	**3.58**	1.08	1.14	1.37	0.91	1.19	**3.58**
Brassica vegetables (cauliflower)	0.04	0.06	0.04	0.14	0.16	0.05	n.d.	**0.19**	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	**0.19**

*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