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

The REACH-IN Project

**15 November 2018**

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## Sector Specific Terminology and Abbreviations

| Plant Protection Product Terminology | REACH Equivalent Terminology / Clarification |
|---|---|
| AI | Active ingredient |
| PPP | Plant protection product |
| Co-formulant | A component of a formulation other than the AI. Also sometimes referred to as an "inert". |
| Formulation | Preparation or mixture |
| Farmer | Professional worker |
| Amateur | Consumer |
| Bystanders | Members of the public potentially exposed during application of a PPP |
| Residents | Members of the public living in the close vicinity of an agricultural field and potentially experiencing long-term exposure to co-formulants in PPP applied to crops |
| Re-entry | A situation in which a worker is entering an area after it has been treated with a PPP |

## Disclaimer

ECPA is making the ECPA 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, ECPA does not guarantee that the tools work error-free. ECPA 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 ECPA OWB and LET. All usage is at the discretion of the user and ECPA 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 or imported in quantities of >10 t/year. For substances meeting the criteria for classification or considered as otherwise being hazardous, a quantitative or qualitative exposure assessment and risk characterisation will be required, covering all relevant identified uses and all life-cycle stages of a substance.

Accordingly, the European Crop Protection Association (ECPA) 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 ECPA REACH-IN. Further information can be found on the ECPA website (http://www.ecpa.eu/information-page/regulatory-affairs/reach).

In the case of professional workers (i.e. farmers) and consumers, an exposure modelling tool (ECPA OWB) has been developed to assess the potential exposure to co-formulants arising from plant protection uses. ECPA 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 chemical safety report (CSR).

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

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


ECPA SpERCs have been developed and are incorporated in the ECETOC TRA since version 2, but can also be utilised in CHESAR, and "manually" in EUSES. The SpERCs are conservative, and are recommended as a first tier environmental risk assessment for the assessment of regional scale impacts, and humans exposed *via* the environment.

To complement the SpERCs, the ECPA has developed the ECPA LET for the specific assessment of potential exposure at the local scale and of secondary poisoning, 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 the use of substances as co-formulants.

# 1. The ECPA 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 to be the minimum required to cover substances used as co-formulants in plant protection products (PPP).

In addition, it describes the link between the Use Descriptors and the activities covered in the ECPA developed REACH-IN exposure modelling tools. 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

This guidance document summarises the Identified Uses of substances as co-formulants in PPP based on ECHA Use Descriptors (ECHA guidance R.12, ECHA 2015).

The use descriptors are provided for the ECPA Generic Exposure Scenarios (Dobe et al. 2017, https://onlinelibrary.wiley.com/doi/full/10.1111/risa.12666) developed by the European Crop Protection Association (ECPA) for the Identified Uses by professional workers (farmers) and consumers (amateurs). It is important to note that for co-formulant uses in PPP, the assignment of Use Descriptors are mainly 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, certain PROCs describing professional activities such as spraying are not representative of the application of a co-formulant in PPP).

The following are typical activities with PPP for which a co-formulant REACH risk assessment may be required:

- handling and spraying of formulations
- handling and sowing of seeds which have been treated
- handling and dispersion of granular formulations (direct application as such to soil).

The various tasks associated with the use of a substance as a co-formulant in PPP have been summarised and collated into the following four Identified Uses and combinations of appropriate Use Descriptors, and while not necessarily covering all possible application methods, 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 | SU1, PROC 8a, PROC 11, ECPA SpERC 8d.2.v3 |
| 2 | Use as a co-formulant in plant protection products, seed and granular applications by professionals | SU1, PROC 8a, PROC 8b, ECPA SpERC 8d.1.v3 |
| 3 | Use as a co-formulant in plant protection products, spray applications by consumers | PC27, ECPA SpERC 8d.2.v3 |
| 4 | Use as a co-formulant in plant protection products, seed and granular applications by consumers | PC27, ECPA SpERC 8d.1.v3 |

Each Identified Use has an associated ECPA 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 | | SU1, PROC 8a, PROC 11, ECPA SpERC 8d.2.v3 |
| Contributing environmental scenario | ECPA SpERC 8d.2.v3 | Spray application of plant protection products containing co-formulants (indoor or outdoor) |
| Contributing worker scenario | PROC 8a | Mixing and loading of plant protection products into delivery equipment |
| Contributing worker scenario | 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 | | SU1, PROC 8a, PROC 8b, ECPA SpERC 8d.1.v3 |
| Contributing environmental scenario | ECPA SpERC 8d.1.v3 | Direct application of plant protection products (granules or treated seeds) containing co-formulants to soil  (indoor or outdoor) |
| Contributing worker scenario | PROC 8a | Mixing and loading of plant protection products into seed treatment or delivery equipment |
| Contributing worker scenario | PROC 8b | Transfer of treated seeds from batch treater into bags |
| Contributing worker scenario | 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 | | PC27, ECPA SpERC 8d.2.v3 |
| Contributing environmental scenario | ECPA SpERC 8d.2.v3 | Spray application of plant protection products containing co-formulants (indoor or outdoor) |
| Contributing consumer scenario | 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 | | PC27, ECPA SpERC 8d.1.v3 |
| Contributing environmental scenario | ECPA SpERC 8d.1.v3 | Direct application of plant protection products (granules or treated seeds) containing co-formulants to soil (indoor or outdoor) |
| Contributing worker scenario | 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. If necessary, these activities need to be covered by specific assessments using standard exposure assessment tools under REACH, e.g. ECETOC TRA, CHESAR or the Advanced REACH Tool.

## 1.2.1  Use Descriptor Entry in IUCLID 6

The following examples are for Use Descriptor entry in IUCLID 6 (version 6.2) Section 3.5.

**Use by Professional Workers**

Contributing activity / technique for the environment

Name of activity / technique

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

Contributing activity / technique for workers

Name of activity / technique

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

Name of activity / technique

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

Product category used
▼ PC 27: Plant protection products

Sector of end use
▼ SU 1: Agriculture, forestry and fishing

Technical function of the substance during use
▼ processing aid
   solvent

Substance supplied to that use in form of
▼ in a mixture

Subsequent service life relevant to this use
no                                          ...  ▼

**Consumers Uses**

Contributing activity / technique for the environment

Name of activity / technique

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

Contributing activity / technique for consumers

Name of activity / technique

Product category (PC)
▼ PC 27: Plant protection products

Technical function of the substance during use
▼ processing aid
   solvent

Substance supplied to this use in the form of
▼ in a mixture

### 1.2.2  Previous Identified Use Compilations

ECPA developed an early compilation of Use Descriptors containing a total of 14 Identified Uses for co-formulants in PPP. These have been consolidated and simplified by recognising the common tasks inherent to each use. This lead to the four Identified Uses described in this guidance document, 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)

And for Consumer Uses:

- 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, the ECPA 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 ECPA REACH-IN group selected also representative values for the input parameters to be used in the tools for a default assessment resulting in reasonable worst-case estimates for worker, consumer and environmental exposures. The use of these tools is highly recommended for the assessment of substances used as a co-formulant in PPP.

The ECPA REACH-IN OWB tool (Mostert et al. 2018, https://doi.org/10.1093/annweh/wxy088, describing version 3.3) 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 aspects of the Identified Uses. These models thus define the scope (tasks and use patterns) for the worker and consumer contributing scenarios. The current version 4.0 of the OWB tool has been upgraded and based on the models published by EFSA for the assessment of exposure of operators, workers, bystanders and residents (EFSA 2014).

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

The ECPA REACH-IN tools are designed to provide output directly linked to the above Identified Uses and ECPA Generic Exposure Scenarios. The following sections describe for each Generic Exposure Scenario the tasks covered by each contributing scenario and Use Descriptor. In particular for the ECPA 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: ECPA SpERC 8d.2.v3 - Spray application of plant protection products containing co-formulants**

The ECPA spray application SpERC (8d.2.v3) considers vapour-pressure dependent direct emissions to soil and/or air and direct emissions to surface water due to spray drift, which for wide dispersive uses are considered only at the regional scale. The SpERC has been implemented in ECETOC TRA.

The SpERC is not intended to provide a definitive estimate of environmental exposure at the local scale, which is calculated with the ECPA LET for the use of a substance as a co-formulant.

The ECPA SpERC, when selected in ECETOC TRA, 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 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, or CHESAR. Furthermore, the ECPA SpERC will be made available as part of a use map file that can be imported into CHESAR 3.3.

Following import of the PEC$_{regional}$ into the LET, the scenario for the spray application of PPP 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 ECPA 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, bystanders and residents.

The ECPA 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 residents and 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 two separate PROC 11 contributing scenarios, one for tractor-mounted spraying, and one for hand-held spraying. However, to keep the exposure scenarios as short as possible, the initial assumption is that the two types of application 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: ECPA SpERC 8d.1.v3- Direct application of plant protection products (granules or treated seeds) containing co-formulants to soil (indoor or outdoor)**

The ECPA treated seed/granular application SpERC (8d.1.v3) considers direct emissions to soil, which for wide dispersive uses are considered only at the regional scale, and has been implemented in ECETOC TRA.

The SpERC is not intended to provide a definitive estimate of environmental exposure at the local scale, which is calculated with the ECPA LET for the use of a substance as a co-formulant.

The ECPA SpERC, when selected in ECETOC TRA, 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 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, CHESAR. Furthermore, the ECPA SpERC will be made available as part of a use map file that can be imported into CHESAR 3.3.

Following import of the $PEC_{regional}$ into the LET, the scenario for application of treated seed/granular PPP 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 seeds and granular PPP which occurs during loading of tractor-mounted broadcast spreader, 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 ECPA 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 8b: Transfer of treated seeds from batch treater into bags**

Description of the activities and technical processes: Transfer of treated seeds from a batch treater into bags.

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.

**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 PPP from manual spreading (by hand), mechanical spreading (belly grinders and push-type rotary spreaders), and from tractor-mounted broadcast spreaders.

The ECPA 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 liquid substances used as solvents, as these can be expected to have evaporated to a significant extent before treated seeds are dispersed. Similarly, only a negligible loading of a liquid in a granule 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: ECPA SpERC 8d.2.v3 - Spray application of plant protection products containing co-formulants**

The ECPA spray application SpERC (8d.2.v3) considers vapour-pressure dependent direct emissions to soil and/or air, which for wide dispersive uses are considered only at the regional scale, and has been implemented in ECETOC TRA.

The SpERC is not intended to provide a definitive estimate of environmental exposure at the local scale, which is calculated with the ECPA LET for the use of a substance as a co-formulant.

The ECPA SpERC when selected in ECETOC TRA is used to estimate the contribution to the regional background concentrations ($PEC_{regional}$) from the use of PPPs by spraying; any local scale PECs calculated in ECETOC TRA 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, CHESAR. Furthermore, the ECPA SpERC will be made available as part of a use map file that can be imported into CHESAR 3.3.

Following import of the $PEC_{regional}$ into the LET, the scenario for the spray application of PPP 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 ECPA 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 ECPA 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: ECPA SpERC 8d.1.v3 - Direct application of plant protection products (granules or treated seeds) containing co-formulants to soil (indoor or outdoor)**

The ECPA treated seed/granular application SpERC (8d.1.v3) considers direct emissions to soil, which for wide dispersive uses are considered only at the regional scale, and has been implemented in ECETOC TRA.

The SpERC is not intended to provide a definitive estimate of environmental exposure at the local scale, which is calculated with the ECPA LET for the use of a substance as a co-formulant.

The ECPA SpERC when selected in ECETOC TRA is used to estimate the contribution to the regional background concentrations ($PEC_{regional}$) from treated seed/granular crop protection uses; any local scale PECs calculated in ECETOC TRA 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, CHESAR. Furthermore, the ECPA SpERC will be made available as part of a use map file that can be imported into CHESAR 3.3.

Following the 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 risk management measures (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 to cover 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 ECPA OWB tool and using the parameters: co-formulant application rate, personal protection (PPE), respiratory protection (RPE).

The above exposure scenario may be scaled using the ECPA Local Environment Tool 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 ECPA Exposure Tool for Operators, Workers and Bystanders (ECPA OWB)

## 2.1 Introduction

A specific tool (ECPA OWB, Mostert et al. 2018) has been developed for the assessment of the potential exposure of operators, workers, residents and bystanders to co-formulants contained in plant protection products (PPP). ECPA OWB covers professional workers and consumers exposed during mixing and loading, spray applications of liquids or dispersion of granular PPP and treated seeds. ECPA OWB is largely based on specific exposure models that have been developed for the authorisation of plant protection products in Europe. These models were developed from dosimetry studies that were conducted during actual field applications of PPP. The ECPA REACH-IN group reviewed these models and selected representative values for the input parameters ensuring the assessment of a reasonable worst case exposure when using the default setting. ECPA OWB therefore provides a more realistic depiction of the actual exposure situation occurring during the use of a substance as a co-formulant in PPP than e.g. ECETOC TRA which lacks parameters specific for applications of PPP. In addition, ECPA OWB allows the user to take account of RMMs such as PPE and 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 of this guidance document cover the use of the ECPA OWB software. Section 2.5 describes the detailed methodology and algorithms used.

## 2.2 General Requirements

- ECPA OWB will run under MS EXCEL 2003 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-Ch9+10_ENV+HH.docx
  - ReportPaste.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

- o Foliar residues at time of re-entry are zero for substances with a vapour pressure of 0.1 Pa or higher.
  - o Re-structuring of CSR Chapter 9 output
- V2.5 (April 2013)
  - o Worst-case scenario for tractor-mounted spraying changes from boom spraying to air-blast if gloves are worn.
- V2.6 (February 2014)
  - o The CSR template has been adapted to the latest CSR template of ECHA (December 2013)
  - o 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)
  - o Integration of the CSR template for LET into the CSR template of OWB
- V3.1 (November 2014)
  - o 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 overprediction of inhalation during M&L is avoided
  - o More queries are introduced to ensure that the worst-case is selected even for unlikely combinations of PPE, use rate, and DNELs
  - o 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)
  - o Generates outputs in .docx format
  - o Hand surface of consumers is 840 cm² instead of 960 cm² for workers, in alignment with REACH guidance R.15
  - o CSR format now based on the ECHA template implemented in IUCLID 5.6
  - o Macro buttons now implemented as Form Buttons, not ActiveX controls for better version-to-version stability
- This version: V4.0 (October 2016)
  - o The BBA model for the assessment of operator, worker and bystander exposure was replaced with the Agricultural Operator Exposure Model (AOEM)
  - o The exposure models for the assessment of activities related to seed treatment were deactivated
  - o CSR format now based on ECHA template implemented in IUCLID 6

## 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.

**(1) Identifier**

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

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

**(2) Substance Data**

- Vapour pressure must be entered in Pascal
- Physical state of the co-formulant. If "liquid", certain scenarios pertaining to dusty formulations will not apply

**(4) Comments**

Use the "Comments" box to enter information on DNEL sources or similar information

| Substance | | |
|---|---|---|
| **Substance data** | | |
| Vapour pressure (room temp.) | | Pa |
| Physical state (room temp.) | solid | |

| **DNELs** | | | **Comments** |
|---|---|---|---|
| Worker, long term, inhalation | | mg/m³ | |
| Worker, long term, dermal | | mg/kg bw/day | |
| General population, inhalation | | mg/m³ | |
| General population, dermal | | mg/kg bw/day | |

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

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

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

- Dermal DNELs must be entered in mg/kg bw/day if based on systemic effects (default)
- Dermal DNELs must be entered in mg/cm² if based on local effects (irritation/ corrosion, sensitisation).

## *2.4.2  Scenario information*

ES # as it appears in the CSR

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

| Scenario information | Professional uses | | | | Consumer uses | |
|---|---|---|---|---|---|---|
| ES no. | PPP GES1<br>Spray application | | PPP GES2<br>Seed and granular application | | PPP GES3 | PPP GES4 |
| ES sub-activity | Tractor-mounted spraying | Hand-held spraying | Seed treatment | Dispersing granules/seeds | Hand-held spraying | Dispersing granules/seeds |
| Application rate (kg/ha) | 1.00 | 1.00 | 100.0% | 20.0 | 1.00 | 20.0 |
| Personal protection (PPE) | **gloves M&L** | no PPE | no PPE | no PPE | | |
| Respiratory protection (RPE) | no RPE | **RPE PF10** | no RPE | no RPE | | |
| Local exhaust ventilation (LEV) | | | *yes* | | | |

Various degrees of PPE and RPE are available from dropdown menus (default is "none"). PPE/RPE will appear in bold font

RPE is not a recommended RMM

PPE/RPE is not available for consumers

## *2.4.3  Results*

The "Results" table will be populated as the necessary hazard and scenario information are entered. The table summarises 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*

**Maximum rate**

Obtains the maximum application rate that is permissible for the current choice of DNELs and RPE/PPE/LEV
You will be prompted to enter the desired target RCR (0 - 1)

**Reset to default**

Restores the default application rates and PPE/RPE/LEV settings. This is helpful for assessing a new scenario for the same substance.

**Report PPP GES**

Copies a summary of the four PPP GESs into a WORD document. The file will be generated in the "Results" folder in the ECPA OWB

**Copy this Page**

Copies the Input & Report page into a WORD document in the "Results" folder. File name is the substance identifier + "_Summary"

**Printout**

Opens the Excel dialogue for printing the "Input & Report" page.

**Create CSR**

Will create a Word document representing Chapter 9 and 10 of the CSR. The file will be generated in the "Results" folder in the ECPA OWB working directory.

**Clear all Inputs**

Will delete all inputs made by the user and restores the default application rates and PPE/RPE/LEV settings.

### 2.4.5  Working with the CSR file

The CSR Chapters 9 and 10 generated by ECPA 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_Ch9+10". **Do not edit any of the files in the "Templates" folder.**

Some system setups result in an error message when the user wants to generate a CSR or other document by using the Macro buttons in the "Input & Result" tab in the OWB tool. To enable the CSR generation functionality in these cases, the properties of the template files need to be modified, by disabling the "Read-only" attribute. The user will have to go to the "Templaes" folder after unpacking the OWB software. This folder contains three Word-file documents. The file properties can be changed by clicking on a file with the right button of the mouse, and select "Properties". In the general tab, you will find a box for the "Read-only" attribute. This box needs to be unchecked. **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, e.g.:

**Environment**

**Conclusion on risk characterisation:**

*The RCRs for the environmental compartments are all <1 and indicate that the potential risk for the environment is adequately controlled under the conditions of this exposure scenario.*

**Workers**

**Conclusion on risk characterisation:**

*The RCRs are all <1 and indicate that the risk for worker health is adequately controlled under the conditions of this exposure scenario.*

### 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 extended Safety Data Sheet (eSDS) or similar documents to facilitate risk communication within the supply chain.

| Contributing Scenarios | Use rate (kg/d) | Dermal exposure [mg/kg bw/day] | Inhalation Exposure (mg/m³) | PPE | RPE | Dermal RCR | Inhalation RCR | Total RCR |
|---|---|---|---|---|---|---|---|---|
| **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. | | | | | | | | |
| **Tractor-mounted spraying** | | | | | | | | |
| PROC 8a: Mixing & loading WP formulation into tractor-mounted tank | 7.38 | 0.633 | 0.0517 | no PPE | no RPE | 0.633 | 0.052 | 0.684 |
| PROC 11: Tractor-mounted boom spraying | | 0.215 | 0.0007 | no PPE | no RPE | 0.215 | 0.001 | 0.216 |
| **PROC 8a+11** | | **0.848** | **0.052** | | | **0.848** | **0.052** | **0.900** |
| **Hand-held spraying** | | | | | | | | |
| PROC 8a: Mixing & loading liquid formulation into knapsack sprayer | 0.13 | 0.376 | 0.001 | no PPE | no RPE | 0.376 | 0.001 | 0.376 |
| PROC 11: Hand-held spraying, indoors (greenhouse) | | 0.074 | 0.449 | no PPE | no RPE | 0.074 | 0.449 | 0.524 |
| **PROC 8a+11** | | **0.450** | **0.450** | | | **0.450** | **0.450** | **0.900** |

Instructions | Input & Report | **PPP GES1** | PPP GES2 | PPP GES3 | PPP GES4 | Granules PHED | Model Info | Foliar Application

## 2.5 *Model Information summary*

### 2.5.1 *Introduction*

Assessment of agrochemical uses

The European Crop Protection Association (ECPA) has developed four plant protection product Generic Exposure Scenarios (PPP GES, Dobe et al. 2017) for assessing human and environmental exposure to non-active substances (co-formulants) used in plant protection products (PPP). The ECPA GES have been built using exposure models that are established in the EU and USA for assessing human and environmental exposure to active substances used in PPP. The models have been adapted to suit the requirements of REACH, e.g. the need for a route-specific external exposure rather than a systemic exposure assessment, and the application of the REACH use descriptor system. Furthermore, they have been pre-populated with representative values for input parameters ensuring a reasonable worst case exposure assessment when the models are used in the default mode.

The following Identified Uses 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 ECPA OWB tool, which incorporates exposure models which are well-established for the safety

assessment of PPP in the EU and the USA. 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 liquid, or powder, 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, worker: 70 kg (EFSA models may use 60 kg)

- Body weight, general population: 60 kg (adult), 10 kg (child)

- Respiratory volume, worker: 10 m³/ 8 h

- Respiratory volume, general population: 20 m³/ 24 h

The most significant exposure determinant in standard PPP exposure models is the use rate (in kg/ha), which can be directly related to the potential exposure to a substance contained in the plant protection product. To minimise "artificial" restrictions on co-formulant uses, the standard PPP exposure models were adapted for use under REACH to output the maximum safe use rate for a defined target RCR. For example, if a target RCR of 0.1 was specified, the maximum use rate which delivers this RCR is calculated iteratively.

The individual models implemented in ECPA 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 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; 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, bystanders and residents.

The current version of the ECPA OWB tool uses the Agricultural Operator Exposure Model (AOEM), which has been jointly developed by PPP regulators and agrochemical companies (Großkopf et al. 2013). The AOEM is based on measured data obtained in exposure studies that have not previously been used in official regulatory exposure models. Studies that were included in the model had to fulfil a number of quality criteria, e.g. studies had to be carried out under Good Laboratory Practice (GLP) and in accordance with OECD Test guidelines and monitor professional agricultural operators following Good Agricultural Practice (GAP). A total of 34 studies were included in AOEM that were conducted between 1994 and 2009 in different European countries of the central and southern zones. These studies covered modern application techniques with vehicle-mounted, vehicle-trailed and self-propelled sprayers and hand-held spray guns and knapsack sprayers, and different types of plant protection product formulations. A variety of crops, such as cereals, potatoes, sugar beet, pomes, citrus and grapevine were covered by the studies.

### 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 "German BBA model" (Lundehn *et al.*, 1992) was widely used in this context

in the past, but has been replaced by a new model for the estimation of Agricultural Operator Exposure (AOEM, Großkopf et al. 2013) adopted in a new EFSA guidance on the assessment of operator exposure and made available as an Excel calculator tool (EFSA 2014).

The studies selected for the development of AOEM were monitoring exposure of workers during a typical working day and considered mixing and loading of different types of plant protection product formulations. Mixing and loading activities covered the filling of a tank and a knapsack, and this included cleaning activities in some cases. The duration of the mixing and loading activities in the studies included in AOEM ranged from 10 to 182 minutes (with a median of 40 minutes) for the filling of tanks and from 17 to 130 minutes (with a median of 30 minutes) for the filling of knapsacks. The amount of product handled during mixing and loading activities depends on the treated crops and the type of equipment used, and the following representative values were considered in AOEM:

- Hand-held application using knapsack sprayers: 1 ha per day for all crops
- Hand-held application using tank sprayers with lances: 4 ha per day for all crops
- Application with vehicle-mounted sprayers: 10 ha per day for high crops, e.g. stone fruit, cane fruit, hops, grapes, tree nuts
- Application with vehicle-mounted sprayers: 50 ha per day for low crops, e.g. cereals, berries, legume vegetables, brassica vegetables

Three distinct formulation types have been considered: liquids, granules and powders.

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 specifically mentioned, the "AOEM" assumes no protective clothes are worn, i.e. workers wear light clothes consisting of T-shirt, shorts and shoes.

The transfers of solid and liquid PPP which occur 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 for these sub-activities is carried forward for risk characterisation as the generic conservative PROC 8a value for this contributing scenario.

**Table 1:** Typical ECPA OWB output table (PROC8a) showing exposure estimates for all variable exposure determinants within the AOEM 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 | 0.253 | 0.0004 | 0.253 |
| | AOEM | Powder (WP) | 0.633 | 0.0517 | **0.684** |
| | AOEM | Granule (WG) | 0.211 | 0.0059 | 0.217 |
| Mixing and loading tractor-mounted/trailed broadcast air-assisted sprayer | AOEM | Liquid | 0.101 | 0.0002 | 0.101 |
| | AOEM | Powder (WP) | 0.253 | 0.0207 | 0.274 |
| | AOEM | Granule (WG) | 0.084 | 0.0024 | 0.087 |
| Mixing and loading hand-held sprayer, outdoors or indoors | AOEM | Liquid | 0.376 | 0.0006 | 0.376 |
| | AOEM | Powder (WP) | 0.092 | 0.0103 | 0.102 |
| | AOEM | Granule (WG) | 0.038 | 0.0003 | 0.039 |

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

A number of established models are available for the assessment of operator exposure to (active) substances in PPP. The "German BBA model" (Lundehn *et al.*, 1992) was widely used in this context in the past, but has been replaced by a new model for the estimation of Agricultural Operator Exposure (AOEM, Großkopf et al. 2013) adopted in a new EFSA guidance on the assessment of operator exposure and made available as an Excel calculator tool (EFSA 2014).

The studies selected for the development of AOEM were monitoring exposure of workers during a typical working day and considered typical spray application techniques and scenarios for outdoor treatment of low and high crops. The equipment covered in the studies consisted of tractor-mounted or tractor-trailed sprayers, self-propelled sprayers and hand-held spray guns and knapsack sprayers. Tractors used for the large-scale treatment of low crops, e.g. cereals or potatoes, were generally equipped with cabins, whereas only half of the sprayers used for the treatment of vineyards and orchards had cabins. The studies covering hand-held knapsack sprayers only investigated applications involving downward spraying, whereas the studies covering tank sprayers with lances investigated only applications involving upward spraying.

The amount of product handled during mixing and loading activities depends on the treated crops and the type of equipment used, and the following representative values were considered in AOEM:

- Hand-held application using knapsack sprayers: 1 ha per day for all crops
- Hand-held application using tank sprayers with lances: 4 ha per day for all crops
- Application with vehicle-mounted sprayers: 10 ha per day for high crops, e.g. stone fruit, cane fruit, hops, grapes, tree nuts
- Application with vehicle-mounted sprayers: 50 ha per day for low crops, e.g. cereals, berries, legume vegetables, brassica vegetables

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 (tank sprayers with lances, knapsack). Unless specifically mentioned, the "AOEM" assumes no protective clothes are worn, i.e. workers wear light clothes consisting of T-shirt, shorts and shoes.

**Table 2:** Typical ECPA 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 | PPE | RPE | Dermal exposure [mg/kg bw/day] | Oral exposure [mg/kg bw/day] | Inhalation exposure [mg/m³] | Total RCR |
|---|---|---|---|---|---|---|---|---|
| Tractor mounted/trailed boom spraying | | | no PPE | no RPE | 0.125 | | 0.001 | 0.021 |
| Tractor mounted/trailed broadcast air-assisted spraying | | | no PPE | no RPE | 0.536 | | 0.023 | 0.092 |
| Hand-held spraying, high-level target, outdoors | AOEM* | | no PPE | no RPE | 0.166 | | 0.026 | 0.030 |
| Hand-held spraying, high-level target, indoors (greenhouses) | AOEM | Liquid | no PPE | no RPE | 0.166 | | 0.026 | 0.030 |
| Worker re-entry (indirect exposure) | EFSA | Liquid | Normal work wear | | 1.800 | | Not assessed | 0.300 |

| Type of equipment and conditions | Model | Formulation type | PPE | RPE | Dermal exposure [mg/kg bw/day] | Oral exposure [mg/kg bw/day] | Inhalation exposure [mg/m³] | Total RCR |
|---|---|---|---|---|---|---|---|---|
| Indirect exposure of residents (children) | EFSA | Liquid | | | 1.094 | 0.009 | 0.002 | 0.368 |
| *AOEM: Agricultural operator exposure model , CRRM: constant rate release model | | | | | | | | |

The models used in addition to the AOEM in Table 2, CRRM, and EFSA are described in the following sections.

### 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 to high targets. Dermal and inhalation exposure to spray mist is assessed using the "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 ECPA 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.

**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:

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

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:

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

where:

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

and

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

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 that evaporation is immediate for substances with a vapour pressure >0.1 Pa.

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 hours 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 assumed to leave the greenhouse.

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

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

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 $t = t_r = 6$h, 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.**
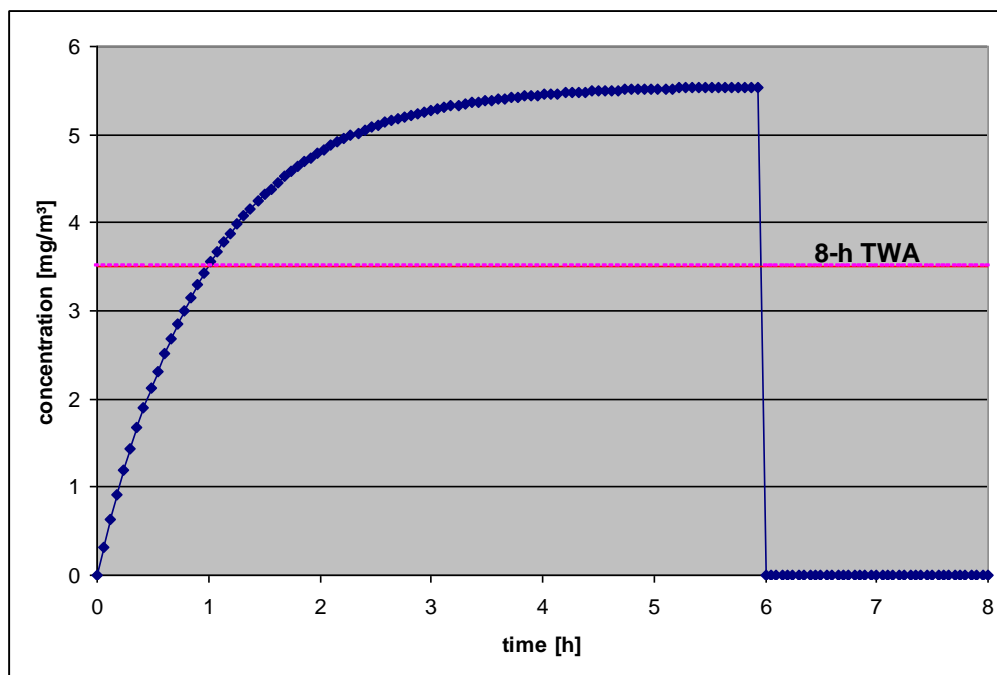


Immediate and complete evaporation of a substance as it is released from the spray nozzle is assumed, when the vapour pressure of a substance is ≥0.1 Pa. For such substances, exposure to vapour is calculated using Equation 8 and added to the exposure to spray calculated with AOEM. These cases are

indicated in output tables as "CRRM", the constant rate release model. For substances with lower vapour pressures, only spray exposure (from the AOEM) is considered relevant.

### 2.5.2.5   *Calculation of Exposure due to Worker Re-entry*

While not explicitly considered in industrial or professional exposure assessments, worker exposure resulting from re-entry to a treated field 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), the DFR is zero 24 h 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. Exposure of workers entering treated areas is predicted using the exposure models and parametrisation proposed by the European Food Safety Agency (EFSA 2014). The following assumptions are made:

- Re-entry exposure is predominantly via the dermal route (contact with the foliage)

- Residues on the foliage depend on:
  - application rate
  - extent of remaining residues from previous applications (assumed to be negligible)
  - the Leaf Area Index (LAI) [total size of foliage compared to surface area]

- Transfer of residues from foliage to the clothes or skin of workers depends mainly on the intensity of contact with the foliage

- Activities with a similar pattern can be grouped and a generic Transfer Coefficient (TC) applied

- The DFR is assumed to be 3 µg.cm$^{-2}$ of foliage.kg$^{-1}$ substance applied.ha$^{-1}$

This figure is published as a highly conservative value in the EFSA guidance (EFSA 2014). Workers re-enter the treated culture shortly after the spray has dried on plant surfaces. Re-entry activities (e.g., pruning) are most common for ornamentals that are treated using hand-held equipment. Thus, the relevant application rate of the hand-held application is adopted for calculation of the DFR.

The DFR is directly proportional to the application rate. As a result, the potential dermal dose (*D*) is calculated using the following equation:

$$D = DFR \cdot TC \cdot WR \cdot AR$$    **Equation 9**

Where:

|  |  |  |
|---|---|---|
| *DFR* = Dislodgeable foliar residues | [µg.cm$^{-2}$] |
| *TC* = Transfer coefficient | [cm$^2$.person$^{-1}$.h$^{-1}$] |
| *WR* = Work rate | [h.day$^{-1}$] |
| *AR* = Application rate | [kg.ha$^{-1}$] |

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:**

Krebs *et al.* (2000) propose in a general approach that a transfer coefficient (TC) of 30000 (cm$^2$/person/h) be used for the transfer of residues from foliage to the clothes or skin of a worker in initial estimates of exposure. This value is considered to represent a worst case for worker exposure, being derived from tasks requiring intensive contact with foliage and representing an unprotected

worker. However, where it is considered that less intensive contact with the foliage will occur, the risk assessment may be refined by the use of alternative transfer coefficients (TC).

Alternative TCs for re-entry activities are published with a wide range (Krieger *et al.*, 1992). It has to be noted that these figures refer to potential transfer coefficients which describe potential dermal exposure. For further estimation of actual dermal exposure, mitigation by ordinary working clothes has to be taken into account. Generally, potential exposure can be assumed to be reduced by 90% when long sleeved shirts and long pants are worn.

In accordance with the approach followed by EUROPOEM II (van Hemmen *et al.* 2002) and the EFSA guidance (EFSA 2014), a representative TC value of 4500 cm$^2$/h is chosen in the default calculations run in the OWB tool. The value will describe a reasonable worst-case for a worker re-entering an outdoor area with treated crops wearing normal work clothes and no further dermal protection (e.g. gloves) and having intensive skin contact with treated foliage.

The skin contact will be mainly with the palmar hand surface, i.e. about 420 cm$^2$. This value is used to estimate the local dose on skin. The bodyweight of a worker is taken as 60 kg.

The following default values and assumptions were used for the calculation of worker exposure occurring during re-entry:

| Variable | Value | Comment |
|---|---|---|
| *DFR* | 3 µg.cm$^{-2}$.kg$^{-1}$.ha$^{-1}$ | Worst case value proposed in the EFSA guidance. |
| *TC* | 4500 cm$^2$.person$^{-1}$.h$^{-1}$ | 75th percentile value proposed in the EFSA guidance. |
| *WR* | 1 ha.day$^{-1}$ | Standard assumption in crop protection exposure assessments for maximum working area for a manual task. |
| *AR* | 1 kg.ha$^{-1}$ (or maximised) | Default application rate (or maximised to a specified RCR). |

### 2.5.2.6   Calculation of Exposure of Residents

While not explicitly considered in industrial and professional exposure assessments, exposure of residents to ingredients of plant protection products is included here as it forms part of the typical risk assessment paradigm used in agrochemical exposure assessments. Exposure of residents 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.

Following the EFSA guidance and the recommendations of the EFSA PPR Panel (2010), four pathways of exposure are considered in the assessment of residential exposure to co-formulants:

- Dermal contact with and inhalation of spray drift at the time of application of PPP
- Inhalation of vapour during and after application of PPP
- Dermal and oral contact with surface deposits
- Dermal and oral contact with treated crops when entering a treated field

Residential exposure for each pathway should be characterised using the 75th percentile exposure estimates for a child and an adult. For the calculation of combined exposure, adding up the 75th percentile exposure estimates may result in an unrealistic worst case exposure, and it is proposed to sum the mean exposure estimates instead (EFSA 2014). The exposure values used in the assessment with the OWB tool were taken from the EFSA guidance, and the respective maximum values were selected.

The OWB tool calculates the worst case mean and 75th percentile exposure estimates for a child and adult member of the general public in accordance with the EFSA guidance, considering four formulation types (wettable powder, granules, wettable granules, soluble and emulsifiable

concentrates). The maximum safe application rate determined for the spray application with hand-held equipment is used in the calculations, and calculations are performed for downward and upward spraying. The final risk assessment is carried out with the combined mean exposure of a child, as this was found to represent the reasonable worst case. The following pathways and routes of exposure are taken into consideration:

| Exposure pathway | Exposure route | Child – calculated exposure estimate | Adult – calculated exposure estimate |
|---|---|---|---|
| Contact with spray drift | Inhalation | Mean, P75 | Mean, P75 |
| | Dermal | Mean, P75 | Mean, P75 |
| Contact with vapour | Inhalation | Highest TWA | Highest TWA |
| Contact with surface deposits | Dermal | Mean, P75 | Mean, P75 |
| | Oral, hand-to-mouth | Mean, P75 | |
| | Oral, object-to-mouth | Mean, P75 | |
| Contact with foliar residues | Dermal | Mean, P75 | Mean, P75 |
| | Oral, hand-to-mouth | Reasonable worst-case | |
| | Oral, object-to-mouth | Reasonable worst-case | |

**Exposure of residents to spray drift**

Inhalation exposure of residents to spray drift is calculated with the following equation:

$$E\text{inh} = \frac{RISDE \times C\text{dil} \times 1000}{BW \times IR}$$ **Equation 10**

Where:

$E_{\text{inh}}$ = Inhalation Exposure                                  mg.m$^{-3}$

$RISDE$ = Maximum inhalation exposure estimate for residents    mL/person

$C\text{dil}$ = Concentration of substance in dilution              kg/L

$BW$ = body weight of resident                                     kg

$IR$ = Inhalation rate of resident                                 m$^3$/day/kg

The concentration of the substance in dilution is calculated by dividing the application rate (in kg/ha) by the minimum water volume for spray application dilution (L/ha).

The dermal exposure of residents to spray drift is calculated with the following equation:

$$E\text{dermal} = \frac{RDSDE \times (1 - LCAF) \times Abs\_dermal\_inuse \times C\text{dil} \times 1000}{BW}$$ **Equation 11**

Where:

$E_{\text{dermal}}$ = Dermal exposure                                   mg.kg.bw$^{-1}$

$RDSDE$ = Maximum dermal exposure estimate for residents        mL/person

$LCAF$ = Adjustment factor for light clothing reducing dermal exposure    none

$Abs\_dermal\_inuse$ = dermal absorption of diluted spray solution    none

$C$dil = Concentration of substance in dilution    kg/L

$BW$ = body weight of resident    kg

The following default values are used in the calculations with the OWB tool in accordance with the EFSA guidance:

| Variable | Value | Comment |
|---|---|---|
| $AR$ | 1 kg.ha$^{-1}$ (or maximised) | Default application rate (or maximised to a specified RCR). |
| $RISDE$ | 0.0013 mL/person | Mean inhalation exposure estimate for upward spraying for a child as provided in EFSA guidance. |
| $RDSDE$ | 1.11 mL/person | Mean dermal exposure estimate for upward spraying for a child as provided in EFSA guidance. |
| $IR$ | 1.07 m$^3$/day/kg | Inhalation rate for a child as provided in EFSA guidance. |
| $DIL$ | 100 L/ha | Minimum water volume used for dilution of PPP to produce spray solution |
| $C$dil | 0.01 kg/L (or maximised) | Calculated by dividing the application rate by the minimum water volume used for dilution. |
| $LCAF$ | 0.18 | Adjustment factor for light clothing reducing the dermal exposure to spray drift, as given in EFSA guidance. |
| $Abs\_dermal\_inuse$ | 1 | For REACH purposes, an external dermal exposure value is calculated, as the dermal absorption is taken considered in the DNEL calculation. Thus, the value is set to 1. |
| $BW$ | 10 kg | Default body weight for a child |

**Exposure of residents to vapours**

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 following vapour drift exposures are added to the spray drift exposure depending on the vapour pressure of the co-formulant:

| Volatility class | Inhalation of vapour drift [mg/m$^3$] |
|---|---|
| Non-volatile (VP $<1 \times 10^{-5}$ Pa) | negligible |
| Semi volatile (VP $\geq 1 \times 10^{-5}$ Pa and $<5 \times 10^{-3}$ Pa) | 0.001 |
| Volatile (VP $>5 \times 10^{-3}$ Pa) | 0.015 |

**Exposure of residents to surface deposits**

A fraction of the applied PPP may be transferred to surfaces in the residential area by spray drift. Residents can experience dermal exposure to these surface deposits. Furthermore, young children may experience also oral exposure to surface deposits. First, children may transfer deposits of PPP to their hands by touching contaminated surfaces and subsequently put their hands into their mouth. Second, children may put objects with contaminated surfaces directly into their mouth. As children experience higher residential exposure to surface deposits in relation to their body weight than adults and this represents the reasonable worst case, the OWB tool uses the exposure of children in the risk characterisation.

The dermal exposure to surface deposits is calculated with the following equation:

$$E\text{dermal} = \frac{AR \times D \times TTR \times TC \times H}{BW}$$  **Equation 12**

Where:

$E_{dermal}$ = Dermal exposure     mg.kg.bw$^{-1}$

$AR$ = Application rate     mg/cm$^2$

$D$ = Drift (percentage of applied PPP)     none

$TTR$ = turf transferable residues     none

$TC$ = transfer coefficient     cm$^2$/h

$H$ = exposure duration     h

$BW$ = body weight     kg

The default values used in the calculations with the OWB tool are as follows in accordance with the EFSA guidance:

| Variable | Value | Comment |
|---|---|---|
| $AR$ | 1 kg.ha$^{-1}$ (or maximised) | Default application rate (or maximised to a specified RCR). |
| $D$ | 18.96% | This is the highest mean drift percentage value for fruit crops given as given in EFSA guidance. |
| $TTR$ | 0.05 or 0.01 | The turf transferable residues is assumed to be 5% for water soluble formulations and 1% for granular formulations according to EFSA guidance. |
| $TC$ | 2600 cm$^2$/h | Transfer coefficient value for surface deposits used for a child according to EFSA guidance. |
| $H$ | 2 hours | Exposure duration for contact with surface deposits according to EFSA guidance. |
| $BW$ | 10 kg | Default body weight for a child |

The potential oral exposure of children due to hand-to-mouth contact is calculated with the following equation:

$$E\text{oral} = \frac{AR \times D \times TTR \times SE \times SA \times Freq \times H}{BW}$$  **Equation 13**

Where:

| | | |
|---|---|---|
| $E_{oral}$ = Oral exposure | | mg.kg.bw$^{-1}$ |
| $AR$ = Application rate | | mg/cm$^2$ |
| $D$ = Drift (percentage of applied PPP) | | none |
| $TTR$ = turf transferable residues | | none |
| $SE$ = saliva extraction factor | | none |
| $SA$ = surface area of the hand in contact with the mouth | | cm$^2$ |
| $Freq$ = frequency of hand-to-mouth contact | | events per hour |
| $H$ = exposure duration | | h |
| $BW$ = body weight | | kg |

The oral exposure of children that may result from the mouthing of objects with contaminated surfaces is calculated with this equation:

$$E\text{oral} = \frac{AR \times D \times DRP \times IgR}{BW} \qquad \textbf{Equation 14}$$

Where:

| | | |
|---|---|---|
| $E_{oral}$ = Oral exposure | | mg.kg.bw$^{-1}$ |
| $AR$ = Application rate | | mg/cm$^2$ |
| $D$ = Drift (percentage of applied PPP) | | none |
| $DRP$ = dislodgeable residues percentage | | none |
| $IgR$ = ingestion rate for mouthing of objects | | cm$^2$ |
| $BW$ = body weight | | kg |

The default values used in the calculations with the OWB tool are as follows in accordance with the EFSA guidance:

| Variable | Value | Comment |
|---|---|---|
| $AR$ | 1 kg.ha$^{-1}$ (or maximised) | Default application rate (or maximised to a specified RCR). |
| $D$ | 18.96% | This is the highest mean drift percentage value for fruit crops given as given in EFSA guidance. |
| $TTR$ | 0.05 or 0.01 | The turf transferable residues is assumed to be 5% for water soluble formulations and 1% for granular formulations according to EFSA guidance. |
| $SE$ | 50% | Default fraction extracted by saliva according to EFSA guidance. |
| $SA$ | 20 cm$^2$ | Default value for surface area of hand put into mouth according to EFSA guidance. |
| $Freq$ | 9.5 | Default value for the number of mouthing events per hour according to EFSA guidance. |

| Variable | Value | Comment |
|---|---|---|
| $H$ | 2 hours | Exposure duration for contact with surface deposits according to EFSA guidance. |
| $DRP$ | 20% | Default value for percentage of dislodgeable residues transferable from objects to mouth according to EFSA guidance. |
| $IgR$ | 25 cm$^2$ | Default value for surface of objects put into mouth (represented by grass) according to EFSA guidance. |
| $BW$ | 10 kg | Default body weight for a child |

**Exposure of residents to foliar residues during entry of treated fields**

Following the exposure scenarios described in the EFSA guidance for the assessment of residential exposure to PPP, residents may enter a treated field shortly after the application of PPP. This may result in dermal exposure of adults and children to foliar residues. Furthermore, children may have oral exposure to these foliar residues as a result of hand-to-mouth contact and mouthing of objects with contaminated surfaces. As children experience the higher residential exposure to foliar residues in relation to their body weight than adults and this represents the reasonable worst case, the OWB tool uses the exposure of children in the risk characterisation.

The dermal exposure to foliar residues during entry of treated fields is calculated in the same way as dermal exposure of workers entering a treated field (Equation 9). The dermal exposure to foliar residues resulting from entry of treated turf is calculated with the following equation:

$$E\text{dermal} = \frac{AR \times TTR \times TC \times H}{BW}$$   **Equation 15**

Where:

$E_{\text{dermal}}$ = Dermal exposure                mg.kg.bw$^{-1}$

$AR$ = Application rate                    mg/cm$^2$

$TTR$ = turf transferable residues            none

$TC$ = Transfer coefficient for entry into treated crops    cm$^2$/h

$H$ = exposure duration                  h

$BW$ = body weight                    kg

The default values used in the calculations with the OWB tool are as follows in accordance with the EFSA guidance:

| Variable | Value | Comment |
|---|---|---|
| $AR$ | 1 kg.ha$^{-1}$ (or maximised) | Default application rate (or maximised to a specified RCR). |
| $TTR$ | 0.05 or 0.01 | The turf transferable residues is assumed to be 5% for water soluble formulations and 1% for granular formulations according to EFSA guidance. The OWB tool currently uses only the higher TTR value in all calculations. |

| Variable | Value | Comment |
|---|---|---|
| $H$ | 0.25 hours | Exposure duration for contact with foliar residues during entry of treated crops according to EFSA guidance. |
| $TC$ | 1794 cm$^2$/h | The EFSA guidance proposes a mean TC value of 5980 cm$^2$/h for adult residents entering treated crops, and suggests to apply a factor of 0.3 to calculate the corresponding TC value for a child. |
| $BW$ | 10 kg | Default body weight for a child |

### 2.5.2.7 Calculation of Exposure of Bystanders

While not explicitly considered in industrial and professional exposure assessments, exposure of bystanders to spray drift 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.

In principle, exposure of bystanders to co-formulants should be assessed in the same way as exposure of residents and for the same pathways and routes of exposure according to the EFSA guidance. However, 95th percentiles of exposure estimates should be used in the calculation of exposure for each single pathway. Furthermore, a combined exposure of bystanders resulting from all pathways should not be considered in the risk assessment. Bystander exposure is secondary to the spray application of plant protection products onto foliage, and it represents an acute exposure occurring over a relatively short period of time. Risk assessments based on acute effects are relatively rare under the REACH regulation and DNELs for acute effects are not derived for the majority of substances. The current version of the OWB tool does not assess the acute exposure of bystanders to substances used as a co-formulant in PPP.

### 2.5.2.8 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 use rate for a given a target RCR.

**Table 3:** Typical ECPA OWB output table showing exposure estimates for correlated tasks across contributing scenarios in GES1.

| Contributing Scenarios | Use rate [kg/d] | Dermal exposure [mg/kg bw/day] | Inhalation Exposure [mg/m³] | Dermal RCR | Inhalation RCR | Total RCR |
|---|---|---|---|---|---|---|
| Tractor-mounted boom spraying | | | | | | |
| PROC 8a: Mixing & loading WP formulation | 7.38 | 0.633 | 0.0517 | 0.633 | 0.052 | 0.684 |
| PROC 11: Tractor-mounted boom spraying | | 0.215 | 0.0007 | 0.215 | 0.001 | 0.216 |
| PROC 8a+11 | | 0.848 | 0.052 | 0.848 | 0.052 | 0.900 |
| | | | | | | |
| Tractor-mounted air-blast spraying | | | | | | |
| PROC 8a: Mixing & loading WP formulation | 2.95 | 0.253 | 0.0207 | 0.253 | 0.021 | 0.274 |
| PROC 11: Tractor-mounted air-blast spraying | | 0.485 | 0.0053 | 0.485 | 0.005 | 0.490 |

| Contributing Scenarios | Use rate [kg/d] | Dermal exposure [mg/kg bw/day] | Inhalation Exposure [mg/m³] | Dermal RCR | Inhalation RCR | Total RCR |
|---|---|---|---|---|---|---|
| PROC 8a+11 | | 0.738 | 0.026 | 0.738 | 0.026 | 0.764 |
| | | | | | | |
| Hand-held spraying | | | | | | |
| PROC 8a: Mixing & loading liquid formulation into knapsack sprayer | 0.13 | 0.376 | 0.001 | 0.376 | 0.001 | 0.376 |
| PROC 11: Hand-held spraying, indoors (greenhouse) | | 0.074 | 0.449 | 0.074 | 0.449 | 0.524 |
| PROC 8a+11 | | 0.450 | 0.450 | 0.450 | 0.450 | 0.900 |

## 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 products or treated seeds. This scenario includes both indoor and outdoor use.

This generic exposure scenario covers the following tasks: the transfer of treated seeds 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 loading of the concentrated PPP into a process tank for seed treatment, the transfer of treated seeds into bags and the loading of treated seeds or granular PPP into delivery equipment. These tasks considered in the "AOEM" and PHED models can be translated into the systematic use descriptor PROC 8a. The latter model is used to assess the handling of granular materials.

Seed treatment is conducted at designated facilities and is an industrial process. Outdoor seed treatment is performed farm-side on a small scale by professionals. The current AOEM model does not support the assessment of seed treatment activities. For the time being, it has been decided to not cover seed treatment activities in the current version 4.0 of the OWB tool. 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.

Exposure emerging from the loading of granular PPP or treated seeds into a hopper is assessed using The Pesticide Handler Exposure Database (PHED, scenario Mixing/Loading Granules)[1] published by the US Environmental Protection Agency (US EPA) and with the following equations:

$$Ederm = \frac{UE_{route} \times AR \times A}{BW}$$

**Equation 16**

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[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)

$$Einh = \frac{UE_{route} \times AR \times A}{RV}$$  **Equation 17**

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   [mg.kg$^{-1}$]

$BW$ = Body weight                                                                       [kg]

$RV$ = Respiratory volume                                                            [m$^3$]

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

| Variable | Value | Comment |
|---|---|---|
| $AR$ | 20 kg.ha$^{-1}$ (or maximised) | Default application rate (or maximised to a specified RCR) |
| $A$ | 1 to 50 ha | Default value depends on application method and equipment |
| $UE_{dermal\_body}$ | 0.1624 mg.kg$^{-1}$ | Unit value per kg handled, no PPE |
| $UE_{dermal\_hand}$ | 0.0041 mg.kg$^{-1}$ | Unit value per kg handled, no PPE |
| $UE_{inhalation}$ | 0.0012 mg.kg$^{-1}$ | Unit value per kg handled, no PPE |
| $BW$ | 60 kg | Value proposed in EFSA guidance |
| $RV$ | 10 m$^3$ | REACH worker default, light work |

The exposure resulting from loading granules/treated seeds into hand-held equipment is included in the PHED model data for the dispersion sub-activity, and is inherently covered in the exposure values in the following contributing scenario 3. Use of working clothes (long-sleeve shirt, long pants, shoes plus socks) is assumed in the PHED exposure predictions.

**Table 4:** Typical ECPA OWB output table (PROC8a) for GES2 showing exposure estimates for three possible tasks, one of which estimates an exposure for liquids or solids. 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 granules/treated seeds | PHED | Solid (GR) | 0.0290 | 0.0411 | 0.070 |
| Mixing and loading granules/seeds, Belly Grinder and "Push-type" Rotary Spreaders | PHED | Solid (GR) | Loading exposure included in contributing scenario 3: delivery and dispersion | | |

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

The activity covered by this scenario is the bagging of treated seeds, which is assumed to be highly dusty. The current AOEM model does not support the assessment of seed treatment activities. For the time being, it has been decided to not cover seed treatment activities in the current version 4.0 of the OWB tool. 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]

Both 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. The activity can be translated into the systematic use descriptor PROC 8a. Dispersion by hand or hand-held equipment may be used to treat an area of up to 1 ha, and tractor-mounted spreaders may be used to treat areas of up to 50 ha per day according to the EFSA guidance.

Exposure from this application type is assessed using The Pesticide Handler Exposure Database (PHED) published by US EPA. 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 in the OWB tool where measured data to account for the presence or absence of gloves are not available.

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 exposure via 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 assessment in the OWB tool.

See the preceding equations (**Equation 16** and **Equation 17**) for calculating exposures from PHED data. The following default values were used in addition to those previously specified:

| Scenario | Variable | Value | Comment |
|---|---|---|---|
| Applicator, Granules by Hand | $UE_{dermal\_body}$ | 688.71 mg.kg$^{-1}$ | Unit value per kg handled, no PPE |
| | $UE_{dermal\_hand}$ | 285.32 mg.kg$^{-1}$ | Unit value per kg handled, no PPE |
| | $UE_{inhalation}$ | 0.4677 mg.kg$^{-1}$ | Unit value per kg handled, no PPE |
| Applicator, Open Cab Solid Broadcast Spreader | $UE_{dermal\_body}$ | 0.0469 mg.kg$^{-1}$ | Unit value per kg handled, no PPE |
| | $UE_{dermal\_hand}$ | 0.0041 mg.kg$^{-1}$ | Unit value per kg handled, no PPE |
| | $UE_{inhalation}$ | 0.0012 mg.kg$^{-1}$ | Unit value per kg handled, no PPE |
| Spreading by hand | $A$ | 1 ha | Area treated by hand application |
| Mechanical, manual | $A$ | 1 ha | Area treated by manually powered equipment |
| Mechanical, powered | $A$ | 50 ha | Area treated by tractor |
| Mechanical or manual spreading | $AR$ | 20 kg.ha$^{-1}$ (or maximised) | Default application rate (or maximised to a specified RCR) |

**Table 5:** Typical ECPA OWB output table (PROC8a) for GES2 showing exposure estimates for four possible tasks associated with the application of solid, granular products. 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 |
|---|---|---|---|---|---|
| Applicator, Granules by Hand | PHED | Solid (GR) | 0.179 | 0.006 | 0.185 |
| Applicator, Open Cab Solid Broadcast Spreader | PHED | Solid (GR) | 0.034 | 0.029 | 0.063 |

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

The mixing and loading as well as dispersion of PPP and treated seeds, are correlated tasks as they are usually carried out in conjunction by the same workers. The table below reports the relevant combined worst-case exposures from the different contributing. Because of the correlation, these combined RCRs are used in the algorithm to maximise the use rate for a given a target RCR.

**Table 6:** Typical ECPA OWB output table showing exposure estimates for correlated tasks across contributing scenarios in GES1.

| Contributing Scenarios | Use rate [kg/d] | Dermal exposure [mg/kg bw/day] | Inhalation Exposure [mg/m³] | Dermal RCR | Inhalation RCR | Total RCR |
|---|---|---|---|---|---|---|
| Dispersion of granules or treated seeds, tractor | | | | | | |
| PROC 8a: Mixing and loading granules (including treated seeds) | | 0.029 | 0.041 | 0.029 | 0.041 | 0.070 |
| PROC 8a: Applicator, open cab solid broadcast spreader | 109.4 | 0.034 | 0.029 | 0.034 | 0.029 | 0.063 |
| PROC 8a+8a | | 0.063 | 0.070 | 0.063 | 0.070 | 0.133 |
| Dispersion of granules or treated seeds | | | | | | |
| PROC 8a: Spreading of granules or treated seeds using belly grinder, including loading of equipment | 2.74 | 0.863 | 0.037 | 0.863 | 0.037 | 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 m²/day) than professional use. The use of PPE by consumers cannot be assumed. These adaptations are applied to the German BBA model (Lundehn *et al*., 1992) for hand-held applications. The AOEM model published by EFSA does not consider consumer exposure to PPP, and it has been decided to predict the exposure with the older German BBA model in the OWB tool.

The use by consumers 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 PPP is considered to be accidental and beyond a reasonable worst-case scenario.

To account for the higher variation in consumer behaviour, the 75th percentile exposure parameters from the "German BBA Model" database are chosen rather than the respective geometric means. Unless specifically mentioned, the "German BBA model" assumes no protective clothes are worn, i.e. consumers wear light clothes consisting of T-shirt, shorts and shoes.

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 75th percentile 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 is considered to cover the latter case.

The outdoor use of PPP by amateurs covers spraying to high targets and a treatment area of up to 200 m². Indoor uses by amateurs will cover much smaller treatment areas. Therefore, the outdoor scenario is considered to provide a worst-case exposure estimate for amateur indoor uses. No separate model calculation is presented for the indoor spraying by amateurs.

**Table 7:** Typical ECPA 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). 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 hand-held sprayer, outdoors | BBA | Liquid | 0.618 | 0.0004 | 0.619 |
| | BBA | Granule (WG) | 0.246 | 0.0003 | 0.247 |
| | BBA | Powder (WP) | 0.618 | 0.0066 | **0.625** |
| Hand-held spraying, high-level target, outdoors | BBA | Liquid | 0.27 | 0.0036 | 0.275 |

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

**Table 8:** 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 [g/d] | Dermal exposure [mg/kg bw/day] | Inhalation Exposure [mg/m³] | Dermal RCR | Inhalation RCR | Total RCR |
|---|---|---|---|---|---|---|
| Task 1: Mixing & loading powder formulation into knapsack sprayer | | 0.6181 | 0.0066 | 0.618 | 0.0066 | 0.625 |
| Task 2: Hand-held spraying, outdoors | 86 | 0.272 | 0.0036 | 0.272 | 0.0036 | 0.275 |
| Task 1 + 2 | | 0.890 | 0.010 | 0.890 | 0.0102 | 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 products 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 use by consumers 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 18 and Equation 19, assuming 100% absorption, as modified below:

$$E_{dermal} = \frac{AR \cdot A \cdot UE_{route}}{BW \cdot Cf}$$    **Equation 18**

$$E_{inh} = \frac{AR \cdot A \cdot UE_{route}}{RV \cdot Cf}$$    **Equation 19**

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 | | [m$^3$] |
| $C_f$ = lb to kg conversion factor | | [kg.lb$^{-1}$] |

The area that can be treated with manual/mechanical dispersion by a consumer is 200 m$^2$ per day. 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 and takes place a maximum once per day.

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[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))

**Table 9:** Typical ECPA 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) | 0.002 | 0.0000 | 0.002 |
| Belly grinders | SOPREA | Solid (GR) | 0.900 | 0.0003 | **0.900** |
| Hand dispersal, spoon | SOPREA | Solid (GR) | 0.015 | 0.0007 | 0.016 |
| Hand dispersal, cup | SOPREA | Solid (GR) | 0.000 | 0.0001 | 0.000 |
| Hand dispersal | SOPREA | Solid (GR) | 0.400 | 0.003 | 0.403 |

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

## 2.6  ECPA 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 ECPA 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 ECPA REACH IN Local Environment Tool (LET) and the ECPA SpERCs
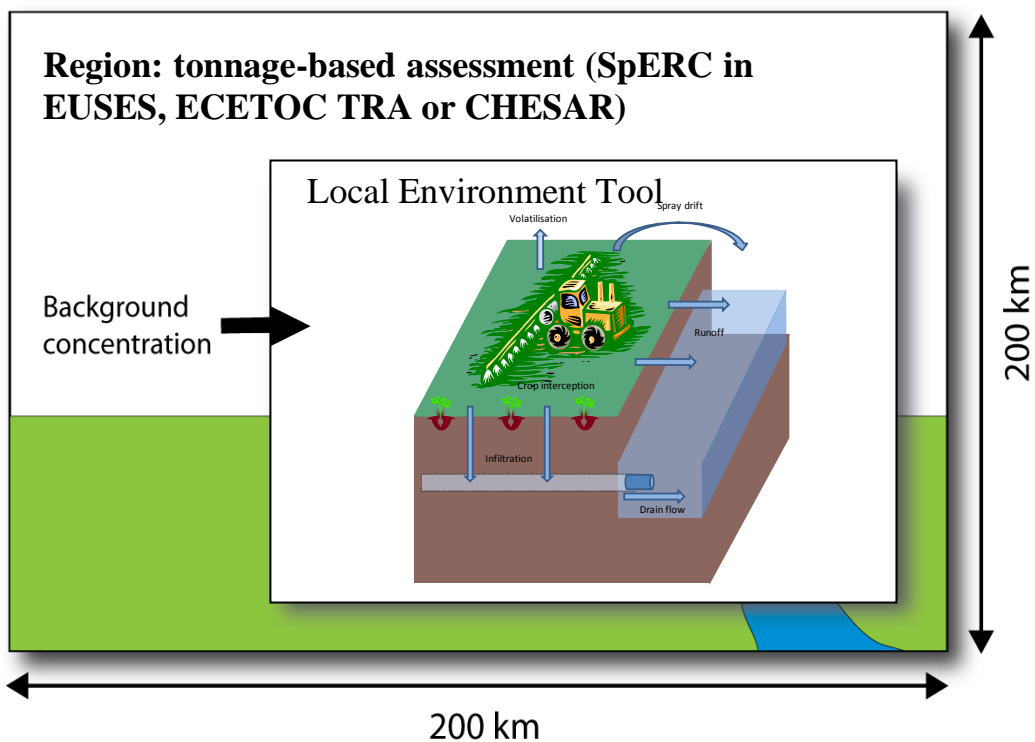
## 3.1 Introduction

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 (PPP) 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 PPP 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 calculate local PECs that are used in the risk characterisation.

Regional PECs should be calculated outside the LET with appropriate tools using the ECPA defined release factors (e.g. ECETOC TRA, EUSES, or CHESAR using the appropriate ECPA SpERCs). The regional PECs can be imported into LET.

The ECPA local environment tool (LET) calculates local-scale exposure estimates and combines local PECs with regional PECs to perform risk characterisations which conform to the requirements of REACH. The LET is a simple spreadsheet which facilitates quantitative local-scale assessments for substances used as a co-formulant in PPP for all REACH relevant environmental compartments (including soil and surface water and secondary poisoning *via* the food chain). Conceptually, a treated 1 hectare (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 3.6 (*Model information & user guidance*).

This scenario design is closely analogous to the established Tier 1 scenario used in the assessment of PPP active substances. 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:
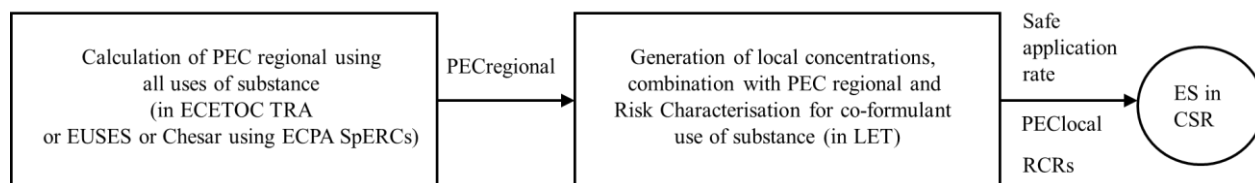


It is foreseen that the LET will have two potential groups of users: Manufacturers/Importers (MI) and Downstream Users (DU). In this context, MI's manufacture or import the substance of interest and register its uses, whilst DU's are plant protection product manufacturers. It is expected that the LET 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 seasonal use rate (in kg/ha) that can be communicated to DU's via the extended Safety Data Sheet (eSDS).

Alternatively, a 'Refinement Options' assessment can be performed. However, due to the level of understanding required and of the very restrictive nature of the Operational Conditions 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, DU's will be able to evaluate whether the existing LET assessment covers their specific representative use pattern of products containing the substance of interest, or refine the assessment (using the Assessment Type: Refinements Options) by scaling, or as part of a 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 ECPA Local Environment Tool (version 3.1) 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 values and PNECs, 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 substance's biodegradability classification to estimate the $DT_{50}$, whereas the $K_{OC}$ value should be entered manually, if the experimental values are known. 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. Selecting one of the options on the QSAR dropdown list for the $K_{OC}$ will allow to calculate the $K_{OC}$ value with an established quantitative structure-activity relationship in accordance with EU-TGD (2003).

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 3.6 (*Model information & user guidance*). A fully documented set of results which can be included in a CSR document is available in the "Exposure Scenario" tab. These tables can be copied into the CSR chapters generated with the OWB tool.

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

## 3.4 'Refinement Options' of the LET

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*

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[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.

*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 application rate, region and crop of application, timing of application and the number and frequency of applications, as well as the interception rate. At the end of a 'Refinement Options' analysis, the RCR values in each environmental compartment are returned based on the specific scenario. In addition, an Estimated Safe Dose is calculated, but the model does not use this as an input at this point. By clicking 'Refine Dose' on the output sheet the model will be re-run for the scenario using the Estimated Safe Dose, should the user wish to explore the RCR values for this (note: the Estimated Safe Dose is calculated using a maximum allowable RCR value of 0.90). Once this has been calculated, there is an option to change the target RCR value on the output screen and selecting "*refine dose*" results in a recalculation of the Estimated Safe Dose for that new RCR value. It should be noted that running the 'Assessment Type: Refinement Options' 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 3.6 (*Model information & user guidance*).

## 3.5 Recommendations for assessment of difficult substances

The LET employs equilibrium partitioning calculations from the EU-TGD. As a result, the same restrictions apply to this tool as to other EU-TGD-based tools such as the ECETOC TRA and CHESAR. Specifically, the tool cannot **necessarily** be used for metals and metal substances, petroleum substances (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 (2017).

### 3.5.1 Assessment of ionisable substances

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

A more detailed discussion on the Environmental Exposure Assessment of Ionisable Organic Compounds is available in the ECETOC Technical Report No. 123 (ECETOC - Publications, 2013).

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 $1\times10^{-10}$ 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 $1\times10^{-10}$ Pa and a $K_{OW}/K_{OC}$ of zero. This is a worst case. The worst case RCRs for each compartment across the results from the two runs constitute the screening level assessment, and the 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 are 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 ECPA 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.

#### 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 10. 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 10: 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 11.

**Table 11: 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) |
|---|---|
| Ready biodegradable | 15 |
| Readily biodegradable, failing 10 day window | 50 |

| Test result | Half-life (days) |
|---|---|
| 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 12 and Table 13.

**Table 12: 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) | Ready 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 13: 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) | Ready 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 20, 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 20**

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 14 to Table 16.

**Table 14: 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) |
|---|---|
| Ready biodegradable | 7.91 |
| Readily biodegradable, failing 10 day window | 26.36 |
| Inherently biodegradable | 79.09 |
| Not biodegradable | 1000 |

**Table 15: Inferred Soil degradation rates at 20 °C reported in the LET on basis of biodegradability screening results and FOCUSsw guidance**

| Kpsoil (L.kg$^{-1}$) | Ready 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 16: Inferred Sediment degradation rates at 20 °C reported in the LET on basis of biodegradability screening results and FOCUSsw guidance**

| Kpsoil ( L.kg$^{-1}$) | Ready 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 21 to Equation 23.

$$Kp_{susp} = K_{OC} \times Foc_{susp} \qquad \textbf{Equation 21}$$

$$K_{susp\text{-}water} = Fwater_{susp} + Fsolid_{susp} \times \frac{Kp_{susp}}{1000} \times RHOsolid \qquad \textbf{Equation 22}$$

$$PNECsediment = \frac{K_{susp\text{-}water}}{RHO_{susp}} \times PNECsw \times 1000 \qquad \textbf{Equation 23}$$

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$^{-1}$] | |
| $K_{susp\text{-}water}$ | Suspended matter-water partition coefficient | [m$^3$.m$^{-3}$] | |
| $PNECsediment$ | Predicted no effect concentration in sediment (wet weight) | [mg.kg$_{wwt}$$^{-1}$] | |

_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.

$$PNECmarine\ water = \frac{PNECsurfacewater}{10} \qquad \textbf{Equation 24}$$

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.

$$PNECmarine\_sediment = \frac{K_{susp\text{-}water}}{RHO_{susp}} \times PNECmarinewater \times 1000 \qquad \textbf{Equation 25}$$

Explanation of symbols

| | | | |
|---|---|---|---|
| $K_{susp\text{-}water}$ | Suspended matter-water partition coefficient | [m$^3$.m$^{-3}$] | Equation 22 |
| $RHOsusp$ | 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 24 |
| $PNECmarine$ $sediment$ | Predicted no effect concentration in marine sediment (wet weight) | [mg.kg wwt$^{-1}$] | |

*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:

$$PNECsed_{dwt} = PNECsed_{wwt} \times CONV_{susp} \qquad \textbf{Equation 26}$$

$$CONV_{susp} = \frac{RHOsusp}{Fsolid_{susp} \times RHOsolid} \qquad \textbf{Equation 27}$$

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 27 |
| $RHOsusp$ | 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 28, in accordance with ECHA R.10 guidance (2008).

$$PNECsoil = \frac{K_{soil\text{-}water}}{RHOsoil} \times PNECsw \times 1000 \qquad \textbf{Equation 28}$$

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 |
| $Ksoil\text{-}water$ | 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}$] |

*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 29**

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}$] | Equation 88 |
| *PNEC$_{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 22). 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 17.

**Table 17: 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 23) |

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 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.

#### 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, 2002). Emission to air is dependent on vapour pressure with the remaining fraction used to estimate emission to soil. These emission fractions are summarised in Table 18 and it is assumed that these emission fractions apply for both indoor and outdoor use. Volatile substances having a vapour pressure of >0.01 Pa at environmental conditions are assumed to volatilise 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, a certain fraction will volatilise and enter the air compartment, and the remaining fraction will enter the soil compartment.

**Table 18: Release to air and soil following volatilisation of sprays (USES 4.0 (RIVM, 2002))**

| 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 | 0.5 |
| >0.000.1-0.001 | 0.2 | 0.8 |
| 0.00001-0.0001 | 0.1 | 0.9 |
| <0.00001 | 0.01 | 0.99 |

In order to determine emission to air under field conditions, the vapour pressure is corrected to a standard temperature of 25 °C using Equation 30.

$$VP(TEMP_{standard}) = VP(TEMP_{test}) \times e^{\frac{H_{0vapor}}{R} \times (\frac{1}{273+TEMP_{test}} - \frac{1}{273+25})} \qquad \textbf{Equation 30}$$

Explanation of symbols

| | | | |
|---|---|---|---|
| $VP(TEMP_{test})$ | Vapour Pressure as give in the data set | [Pa] | User input |
| $H_{0vapor}$ | Enthalpy of vaporisation | [J/mol] | $5 \times 10^4$ |
| $R$ | Gas constant | [Pa.m$^3$.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 17). 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 19) (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 19: 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 ECPA LET and are summarised in Table 20. 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 20: 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 |
| 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.

$$Soil\ Loading = AR \times (1 - F_{air}) \times (1 - F_{crop}) \qquad \textbf{Equation 31}$$

Explanation of symbols

| | | | |
| --- | --- | --- | --- |
| *AR* | Application rate for co-formulant | [g.ha$^{-1}$] | User input |
| $F_{crop}$ | Fraction of interception by crop (refinement option) | [-] | Table 20 |
| $F_{air}$ | Emission factor to air due to volatilisation of spray droplets (spray only) | [-] | Table 18 |
| *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 air 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 17), 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 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 32**

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}$$^{-3}$] | 1700 |
| $Soil\ Loading$ | Soil loading of the co-formulant | [g.ha$^{-1}$] | Equation 31 |
| $10000$ | Area of 1 hectare | [m$^2$] | |
| $Csoil_{initial}$ | Initial concentration in soil | [mg.kg$_{wwt}$$^{-1}$] | |

### 3.6.2.7 Maximum concentration in soil

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

$$Csoil_{max} = Csoil_{initial}$$  **Equation 33**

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 34, losses due to volatilisation are calculated according to Equation 35 and losses due to leaching are calculated according to Equation 36. The equations describing loss processes are in accordance with ECHA guidance R.16.

$$kbio_{soil} = \frac{ln\ 2}{DT_{50}bio_{soil}}$$  **Equation 34**

Explanation of symbols

| | | | |
|---|---|---|---|
| $DT_{50}bio_{soil}$ | Half-life for biodegradation in bulk soil at 12 °C | [d] | Equation 20 |
| $kbio_{soil}$ | first order rate constant for biodegradation in bulk soil | [d$^{-1}$] | |

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

**Equation 35**

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 |
| $K_{air-water}$ | Air-water equilibrium distribution constant | [m$^3$.m$^{-3}$] | Equation 44 |
| $K_{soil-water}$ | Soil-water partitioning coefficient | [m$^3$.m$^{-3}$] | Equation 42 |
| $DEPTH_{soil}$ | Mixing depth of soil | [m] | 0.2 |
| $k_{volat}$ | Pseudo first-order rate constant for volatilisation from soil | [d$^{-1}$] | |

$$k_{leach} = \frac{F\,inf_{soil} \times RAIN_{rate}}{K_{soil-water} \times DEPTH_{soil}}$$

**Equation 36**

Explanation of symbols

| | | | |
|---|---|---|---|
| $Finf_{soil}$ | Fraction of rain water that infiltrates into soil | [-] | 0.25 |
| $RAINrate$ | Rate of wet precipitation (700 mm/year) | [m.d$^{-1}$] | 1.92 x 10$^{-3}$ |
| $K_{soil-water}$ | Soil-water partitioning coefficient | [m$^3$.m$^{-3}$] | Equation 42 |
| $DEPTH_{soil}$ | Mixing depth of soil | [m] | 0.2 |
| $k_{leach}$ | Pseudo-first order rate constant for leaching from soil layer | [d$^{-1}$] | |

The overall rate constant for these removal processes is given in Equation 37.

$$k = k_{volat} + k_{leach} + kbio_{soil}$$

**Equation 37**

Explanation of symbols

| | | | |
|---|---|---|---|
| $k_{volat}$ | Pseudo-first order rate constant for volatilisation from soil | [d$^{-1}$] | Equation 35 |
| $k_{leach}$ | Pseudo-first order rate constant for leaching from top soil | [d$^{-1}$] | Equation 36 |
| $kbio_{soil}$ | Pseudo-first order rate constant for biodegradation in soil | [d$^{-1}$] | Equation 34 |
| $k$ | First order rate constant for removal from top soil | [d$^{-1}$] | Equation 37 |

The maximum concentration in soil following multiple applications is calculated with Equation 38.

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

**Equation 38**

Explanation of symbols

| | | | |
|---|---|---|---|
| $Csoil_{initial}$ | Initial concentration in soil | [mg.kg$_{wwt}$$^{-1}$] | **Error! Reference source not found.** |
| $k$ | First order rate constant for removal from top soil | [d$^{-1}$] | Equation 37 |
| $App\,Int$ | Application interval | [d] | User input |
| $Napp$ | Number of application events | [-] | User input |
| $Csoil_{max}$ | Maximum concentration in soil | [mg.kg$_{wwt}$$^{-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:

$$TWACsoil(t) = Csoil_{max} \times \frac{(1 - e^{(-k \times t)})}{(k \times t)}$$

**Equation 39**

Explanation of symbols

| | | | |
|---|---|---|---|
| $Csoil_{max}$ | Maximum concentration in soil | [mg.kg$_{wwt}$$^{-1}$] | Equation 38 or Equation 34 |
| $k$ | First order rate constant for removal from top soil | [d$^{-1}$] | Equation 37 |
| $t$ | Time period | [d] | Soil: 30<br>Secondary poisoning: 180 |
| $TWACsoil(t)$ | Time weighted average concentration in soil, over a period t | [mg.kg$_{wwt}$$^{-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 40), rather than the 28 days used by default by FOCUS (2003).

$$Clocal_{soil} = TWACsoil( 30d )$$

**Equation 40**

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. This is discussed in more detail in Section 3.6.4.

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

**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.

The concentration in porewater is calculated from the concentration in soil and the soil-water partitioning coefficient. For the secondary poisoning assessment the time weighted average at 180 days is used. The soil-water partitioning coefficient is calculated according to Equation 42.

$$K_{soil\text{-}water} = Fair_{soil} \times K_{air\ water} + Fwater_{soil} + Fsolid_{soil} \times \frac{Kp_{soil}}{1000} \times RHOsolid \qquad \textbf{Equation 42}$$

Where:

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

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

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

Explanation of symbols

| | | | |
|---|---|---|---|
| $VP(TEMP_{env})$ | 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$^{-1}$] | |
| $K_{air\text{-}water}$ | Air-water partitioning coefficient | [-] | |
| $Kpsoil$ | Solids-water partition coefficient in soil | [L.kg$^{-1}$] | |
| $K_{soil\text{-}water}$ | 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.

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

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

Explanation of symbols

| | | | |
|---|---|---|---|
| $VP(TEMP_{test})$ | Vapour Pressure at test temperature | [Pa] | User input |
| $H_{0vapor}$ | Enthalpy of vaporisation | [J.mol$^{-1}$] | $5 \times 10^4$ |
| $R$ | 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$^{-1}$] | $1 \times 10^4$ |
| $TEMP_{test}$ | 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.

$$C_{soil\ porewater} = \frac{C_{soil\ wwt} \times RHOsoil}{K_{soil-water} \times 1000} \qquad \textbf{Equation 48}$$

Explanation of symbols

| | | | |
|---|---|---|---|
| $K_{soil-water}$ | 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 41 |
| $C_{soil\ porewater}$ | 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 22. For the LET 'Default' assessment, the spray drift value for one application to 'fruit (late)' was selected (see Table 17). 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 21 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 21: 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 ECPA LET (Table 22).

**Table 22: 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)** pome / stone fruit, (early) | 3 | 29.2 | 25.5 | 24.0 | 23.6 | 23.1 | 22.8 | 22.7 | 22.2 |
| **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.

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

Explanation of symbols

| | | | |
|---|---|---|---|
| *AR* | Equivalent application rate for co-formulant | [g.ha$^{-1}$] | User input |
| *Drift %* | Drift percentage | [%] | Table 22 |
| *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 31.

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).

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

**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 31 |
| *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.

$$Eq\ Rate\ Runoff\ Event = Eq\ Rate\ Runoff\ Final \times e^{(-4 \times \frac{ln(2)}{DT50soil})}$$

**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 23. For the LET 'Default' assessment parameterisation, the worst-case runoff value of 5% for 'North Europe, Oct – Feb' has been assumed (see Table 17), giving a worst-case assessment of exposure via runoff. The region and season of application can be defined by selecting 'Refinement option'.

**Table 23: 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.

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

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 23 |
| *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).

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

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.

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

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

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.

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

$$Input_{sed}(app) = 0 \qquad\qquad \textbf{Equation 57}$$

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$^{-2}$] | |

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

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

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.

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

$$Mass_{sed}(0) = Input_{sed}(app) = 0 \qquad \text{\textbf{Equation 61}}$$

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.

$$Mass_{sw}\ int_{available}(0) = \frac{Mass_{sw}\ int(0)}{Dist\ Coeff} \qquad \text{\textbf{Equation 62}}$$

$$Mass_{sw}\ int_{unavailable}(0) = Mass_{sw}\ int(0) - Mass_{sw}\ int_{available}(0) \qquad \text{\textbf{Equation 63}}$$

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.

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

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

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.

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

**Equation 66**

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

**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.

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

$$Mass_{sw}\ int_{unavailable}(i) = Mass_{sw}\ int(i) - Mass_{sw}\ int_{available}(i)$$ **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:

$$\begin{aligned} Mass_{sw}(i) = Mass_{sw}\ int\ unavailable(i) + \\ (Mass_{sw}\ int\ available(i) + Mass_{sed}\ int(i)) \times Fwaterphase_{runoff} \end{aligned}$$ **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.

$$Clocal_{SW}(i) = \frac{Mass_{sw}\,int \times 100}{Water\ Depth}$$

**Equation 72**

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

**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 then used in the risk characterisation ratios for surface water and sediment (see Section 3.6.5).

### 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 72 and Equation 73. 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 74 and Equation 75 will be worst-case.

$$Clocal_{marine\,water} = \frac{Clocal_{SW}}{10}$$

**Equation 74**

$$Clocal_{marine\,sed\,(dwt)} = \frac{Clocal_{sed\,(dwt)}}{10}$$

**Equation 75**

Explanation of symbols

| | | | |
|---|---|---|---|
| $Clocal_{sw}$ | Maximum freshwater concentration | [µg.L$^{-1}$] | Equation 72 |
| $Clocal_{sed\,(dwt)}$ | Maximum freshwater sediment concentration (dry weight) | [mg.kg$_{dwt}$$^{-1}$] | Equation 73 |
| $Clocal_{marine\,water}$ | Local marine water concentration | [µg.L$^{-1}$] | |
| $Clocal_{marine\,sed\,(dwt)}$ | Local marine sediment concentration (dry weight) | [mg.kg$_{dwt}$$^{-1}$] | |

### 3.6.4 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) <u>and</u> 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 78 to Equation 85. 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 76.

$$\log BCF_{fish} = 0.85 \times \log Kow - 0.70 \qquad \textbf{Equation 76}$$

For substances with a log $K_{ow}$ higher than 6, Equation 77 is used:

$$\log BCF_{fish} = -0.20 \times \log Kow^2 + 2.74 \times \log Kow - 4.72 \qquad \textbf{Equation 77}$$

Explanation of symbols

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

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 24.

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

**Table 24: 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 $PEC_{\text{surface water}}$, bioconcentration in fish and the biomagnification factor (Equation 78). This is the standard approach in the assessment of active substances in PPP.

$$PEC_{oral, predator} = PEC_{sw} \times BCF_{fish} \times BMF_1 \qquad \textbf{Equation 78}$$

Where:

$$PEC_{sw} = \frac{Clocal_{sw}}{1000} + PECregional_{sw(dissolved)} \qquad \textbf{Equation 79}$$

Explanation of symbols

| Symbol | Description | Units | Notes |
|---|---|---|---|
| $PEC_{sw}$ | PEC in surface water at local scale | $[mg.L^{-1}]$ | |
| $Clocal_{sw}$ | 21-day TWA surface water concentration | $[\mu g.L^{-1}]$ | |
| $PECregional_{sw\ (dissolved)}$ | 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 76 and Equation 77) |
| $BMF_1$ | Biomagnification factor in fish | $[-]$ | Table 24 |
| $PEC_{oral,\ predator}$ | 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 78 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 80).

$$PEC_{oral,\ predator} = 0.5 \times (PEC_{sw} + PECregional_{sw(dissolved)}) \times BCF_{fish} \times BMF \qquad \textbf{Equation 80}$$

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

$$PEC_{oral,\ marine predator} = PEC_{mw} \times BCF_{fish} \times BMF_1 \qquad \textbf{Equation 81}$$

Where:

$$PEC_{mw} = \frac{Clocal_{mw}}{1000} + PECregional_{mw(dissolved)} \qquad \textbf{Equation 82}$$

Explanation of symbols

| Symbol | Description | Units |
|---|---|---|
| $PEC_{mw}$ | PEC in marine water at local scale | $[mg.L^{-1}]$ |
| $Clocal_{mw}$ | 21-day TWA marine water concentration | $[\mu g.L^{-1}]$ |

| | | | |
|---|---|---|---|
| $PECregional_{mw\,(dissolved)}$ | 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}$$^{-1}$] | Measured or estimated from log K$_{ow}$ (Equation 76 and Equation 77) |
| $BMF_1$ | Biomagnification factor in fish | [-] | Table 24 |
| $PEC_{oral,\,marine\,predator}$ | Predicted environmental concentration in food | [mg.kg$_{wet\,fish}$$^{-1}$] | |

Equation 82 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 PEC's 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 83).

$$PEC_{oral,marine\,predator} = 0.5 \times ( PEC_{mw} + PECregional_{mw(dissolved)} ) \times BCF_{fish} \times BMF_1 \qquad \textbf{Equation 83}$$

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 84).

$$PEC_{oral,top\,predator} = PEC_{mw} \times BCF_{fish} \times BMF_1 \times BMF_2 \qquad \textbf{Equation 84}$$

Explanation of symbols

| | | | |
|---|---|---|---|
| $PEC_{mw}$ | 21-day TWA PEC in marine water at local scale | [mg.L$^{-1}$] | Equation 82 |
| $BCF_{fish}$ | Bioconcentration factor for fish on wet weight basis | [L.kg $_{wet\,fish}$$^{-1}$] | Measured or estimated from log K$_{ow}$ (Equation 76 and Equation 77) |
| $BMF_1$ | Biomagnification factor in fish | [-] | Table 24 |
| $BMF_2$ | Biomagnification factor in predator | [-] | Table 24 |
| $PEC_{oral,\,marine\,predator}$ | Predicted environmental concentration in food | [mg.kg$_{wet\,fish}$$^{-1}$] | |

It is assumed for top predators that they mainly prey on organisms from the regional marine environment rather than the local scale. Therefore, where regional PEC's 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 85).

$$PEC_{oral,top\,predator} = ( 0.1 \times PEC_{mw} + 0.9 \times PECregional_{mw(dissolved)} ) \times BCF_{fish} \times BMF_1 \times BMF_2 \qquad \textbf{Equation 85}$$

### 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 87 and Equation 91. If experimental data are not available, bioconcentration in earthworms can be estimated according to Equation 86 described by Jager (1998).

$$BCF_{earthworm} = \frac{(0.84 + 0.012 \times K_{ow})}{RHO_{earthworm}} \qquad \textbf{Equation 86}$$

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 | $[L.kg_{wet\ earthworm}^{-1}]$ | |

### 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_predator is calculated using Equation 87.

$$PEC_{oralpredator} = C_{earthworm} =$$
$$\frac{BCF_{earthworm} \times PEC_{porewater,sec.\ poisoning} + PEC_{soil,sec.\ poisoning} \times F_{gut} \times CONV_{soil}}{1 + F_{gut} \times CONV_{soil}} \qquad \textbf{Equation 87}$$

Where:

$$CONV_{soil} = \frac{RHO_{soil}}{F_{solid} \times RHO_{solid}} \qquad \textbf{Equation 88}$$

$$PEC_{porewater,sec.\ poisoning} = C_{soil\ porewater} + \left( \frac{PEC_{regionalagric\ soil} \times RHO_{soil}}{Ksoilwater \times 1000} \right) \qquad \textbf{Equation 89}$$

$$PEC_{soil,sec.\ poisoning} = TWAC_{soil(180d)} + PEC_{regionalagric.\ soil} \qquad \textbf{Equation 90}$$

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 86) |
| $PEC_{porewater,\ sec.\ poisoning}$ | Predicted environmental concentration in porewater at local scale for secondary poisoning | $[mg.L^{-1}]$ | Equation 89 |
| $PEC_{soil,\ sec.\ poisoning}$ | Predicted environmental concentration in soil at local scale for secondary poisoning | $[mg.kg_{wwt}^{-1}]$ | Equation 90 |

| $F_{gut}$ | 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 88 |
| $RHO_{soil}$ | 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 41 |
| $C_{earthworm}$ | 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 87 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 91).

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

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

**Equation 91**

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 PEC and RCR Calculations

### 3.6.5.1 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). ECPA 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 92 to Equation 96. Where regional concentrations are not available, the $PEC_{compartment}$ = $Clocal_{compartment}$.

_PEC Fresh Water (Pelagic)_

$$PECsw = Clocal_{sw} + PECregional_{sw}$$  **Equation 92**

Explanation of symbols

| | | | |
|---|---|---|---|
| $PECregional_{sw}$ | Freshwater concentration at the regional scale | $[\mu g.L^{-1}]$ | Calculated outside the LET |
| $Clocal_{sw}$ | Maximum local freshwater concentration | $[\mu g.L^{-1}]$ | Equation 72 |
| $PECsw$ | Predicted environmental concentrations in freshwater | $[\mu g.L^{-1}]$ | |

_PEC Fresh Water (Sediment)_

$$PECsed = Clocal_{sed} + PECregional_{sed}$$  **Equation 93**

Explanation of symbols

| | | | |
|---|---|---|---|
| $PECregional_{sed}$ | Freshwater sediment concentration at the regional scale (dry weight) | $[\mu g.kg_{dwt}^{-1}]$ | Calculated outside the LET |
| $Clocal_{sed}$ | Maximum local freshwater sediment concentration (dry weight) | $[\mu g.kg_{dwt}^{-1}]$ | Equation 73 |
| $PECsed$ | Predicted environmental concentrations in freshwater sediment (dry weight) | $[\mu g.kg_{dwt}^{-1}]$ | |

_PEC Marine Water (Pelagic)_

$$PECmarinewater = Clocal_{marinewater} + PECregional_{marinewater}$$  **Equation 94**

Explanation of symbols

| | | | |
|---|---|---|---|
| $PECregional_{marine\ water}$ | Marine water concentration at the regional scale | $[\mu g.L^{-1}]$ | Calculated outside the LET |
| $Clocal_{marine\ water}$ | Local marine water concentration | $[\mu g.L^{-1}]$ | Equation 74 |
| $PECmarine\ water$ | Predicted environmental concentration in marine water | $[\mu g.L^{-1}]$ | |

*PEC Marine Water (Sediment)*

$$PECmarine\ sediment = Clocal_{marine\ sediment} + PECregional_{marine\ sediment}$$   **Equation 95**

Explanation of symbols

| | | | |
|---|---|---|---|
| $PECregional_{marine\ sediment}$ | Marine sediment concentration at the regional scale (dry weight) | $[\mu g.kg_{dwt}^{-1}]$ | Calculated outside the LET |
| $Clocal_{marine\ sediment}$ | Local marine sediment concentration (dry weight) | $[\mu g.kg_{dwt}^{-1}]$ | Equation 75 |
| $PECmarine\ sediment$ | Predicted environmental concentration in marine sediment (dry weight) | $[\mu g.kg_{dwt}^{-1}]$ | |

*PEC Soil*

$$PECsoil = Clocal_{soil} + PECregional_{agric.soil}$$   **Equation 96**

Explanation of symbols

| | | | |
|---|---|---|---|
| $PECregional_{agric.soil}$ | Agricultural soil concentration at the regional scale (dry weight) | $[\mu g.kg_{dwt}^{-1}]$ | Calculated outside the LET |
| $Clocal_{soil}$ | Local soil concentration (30 day TWA) (dry weight) | $[\mu g.kg_{dwt}^{-1}]$ | Equation 40 |
| $PECsoil$ | Predicted environmental concentration in soil (dry weight) | $[\mu g.kg_{dwt}^{-1}]$ | |

*3.6.5.2   RCR calculations*

The risk characterisation ratios (RCRs) for each relevant environmental compartment are calculated using Equation 97.

$$RCR_{compartment} = \frac{PEC_{compartment}}{PNEC_{compartment}}$$   **Equation 97**

Explanation of symbols

| | | | |
|---|---|---|---|
| $PEC_{compartment}$ | Predicted environmental concentrations in environmental compartment | | Section 3.6.5.1 |
| $PNEC_{compartment}$ | Predicted no environmental concentrations in environmental compartment | | User input |
| $RCR_{compartment}$ | Risk Characterisation Ratio in environmental compartment | $[-]$ | |

### 3.6.6 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 98 (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.

$$SafeDose_{compartment} = \left( \frac{AR}{RCR_{compartment} - \dfrac{PEC\,Reg_{compartment}}{PNEC_{compartment}}} \right) \times \left( TargetRCR - \frac{PEC\,Reg_{compartment}}{PNEC_{compartment}} \right)$$

**Equation 98**

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 99).

$$PEC\,Reg_{compartment} = PECregional_{compartment}$$

**Equation 99**

For aquatic and terrestrial predators, the safe dose is calculated using Equation 100 to Equation 104. Again, the maximum dose acceptable for the most sensitive environmental compartment for the substance assessed is reported as the estimated safe dose.

$$SafeDose_{compartment} = \left( \frac{AR}{RCR_{local\,concentraion}} \right) \times Targ\,etRCR_{local\,concentraion}$$

**Equation 100**

Where:

$$RCR_{local\,concentration} =$$

$$\left( F_{local\,diet} \times \frac{PEC\,Local_{compartment}}{PNEC_{compartment}} \right) - \left( F_{local\,diet} \times \frac{PEC\,Background_{compartment}}{PNEC_{compartment}} \right)$$  **Equation 101**

$$Target RCR_{local\,concentration} =$$

$$TargetRCR -$$

$$\left( F_{local\,diet} \times \frac{PEC\,background_{compartment}}{PNEC_{compartment}} \right) - \left( F_{regional\,diet} \times \frac{PEC\,Reg_{compartment}}{PNEC_{compartment}} \right)$$  **Equation 102**

Explanation of symbols

| | | | |
|---|---|---|---|
| $AR$ | Application rate for co-formulant | [kg.ha$^{-1}$] | User input |
| $RCR_{local\,concentration}$ | Local concentration RCR | [-] | Equation 101 |
| $TargetRCR_{local\,concentration}$ | Local concentration RCR target | [-] | Equation 102 |
| $F_{local\,diet}$ | Fraction of diet from local scale | [-] | Terrestrial, freshwater and marine water predator = 0.5 <br> 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 <br> 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 103 to Equation 113. 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:

$$PEC\ Background_{compartment} = PECregional_{oral,predator}$$ **Equation 103**

$$PEC\ \mathrm{Re}\,g_{compartment} = PECregional_{oral,predator}$$ **Equation 104**

$$PECregional_{oral,predator} = PECregional_{sw\,ormw(dissolved)} \times BCF_{fish} \times BMF_1$$ **Equation 105**

Marine top predator:

$$PEC\ Background_{compartment} = PECregional_{oral,toppredator}$$ **Equation 106**

$$PEC\ \mathrm{Re}\,g_{compartment} = PECregional_{oral,toppredator}$$ **Equation 107**

$$PECregional_{oral,toppredator} = PECregional_{mw(dissolved)} \times BCF_{fish} \times BMF_1 \times BMF_2$$ **Equation 108**

Terrestrial Predator:

$$PEC\ Background_{compartment} = PECregional_{oral,predator}$$ **Equation 109**

For the calculation of background exposure of terrestrial predators at the local scale (Equation 109), the Regional$_{porewater}$ is calculated directly from the regional PEC in agricultural soil (Equation 110).

$$\mathrm{Re}\,gional_{porewater} = \frac{PEC_{regionalagric.soil} \times RHO_{soil}}{Ksoil\ water \times 1000}$$ **Equation 110**

$$PEC\ \mathrm{Re}\,g_{compartment} = PECregional_{oral,predator}$$ **Equation 111**

For the calculation of exposure of terrestrial predators at the regional scale (Equation 111) the Regional$_{porewater}$ is taken directly as the regional PEC in porewater of agricultural soil (Equation 112).

$$\mathrm{Re}\,gional_{porewater} = PECregional_{agric.soil\ porewater}$$ **Equation 112**

$$PEC_{oralpredator} = \frac{BCF_{earthworm} \times \mathrm{Re}\,gional_{porewater} + \mathrm{Re}\,gional_{agric.soil} \times F_{gut} \times CONV_{soil}}{1 + F_{gut} \times CONV_{soil}}$$ **Equation 113**

## 3.7 Environmental regional model: ECPA 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 ECPA to allow suppliers to calculate regional exposure to co-formulants. This can be done either using ECETOC TRA which has the SpERCs directly implemented, or by transferring the relevant release factors into EUSES. An upload file, facilitating use of the ECPA SpERCs within CHESAR, is also available.

### 3.7.1 Scope of the ECPA SpERCs

The ECPA 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 ECPA 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 ECPA 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 ECPA 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 ECPA 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 ECPA 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.v3. 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 ECPA SpERC for spray application of PPP.

### 3.7.2  Tonnage split between the ECPA 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.v3).

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 ECPA 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.v3; an anti-freeze could be mostly assigned to SpERC 8d.2.v3. 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.v3) and 25% to granule (SpERC 8d.1.v3) 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 ECPA 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 ECPA SpERCs to be defined in both 'manual' and 'batch' mode.

In manual mode it is necessary to select the following options in the "INTERFACE" sheet:

| Option | Input range* | Selection |
|---|---|---|
| Fraction of tonnage to region | F114:F128 | 0.1 |
| Use ERC or SpERC as release estimation approach | G114:G128 | SpERC |
| ERC (mandatory in all cases as use descriptor) | H114:H128 | ERC 8d |
| Industry sector for SpERC | J114:J128 | ECPA |
| SpERC | K114:K128 | ECPA SpERC 8d.1.v3 |
| | | ECPA SpERC 8d.2.v3 |

*ECETOC TRA, Version 3.1

In order to run the tool with the ECPA SpERC in batch mode it is necessary to select the following options in the relevant "datasheet" column:

| 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 |
| Industry sector for SpERC | Row 82 | ECPA |
| SpERC | Row 83 | ECPA SpERC 8d.1.v3 |
| | | ECPA SpERC 8d.2.v3 |
| Select approach SpERC | Row 103 | TRUE |

*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 ECPA SpERCs in CHESAR

**How to load the ECPA SpERCs**

In order to use the ECPA SpERCs within the CHESAR tool it is first necessary to download the ECPA SpERC upload files from the ECPA website.
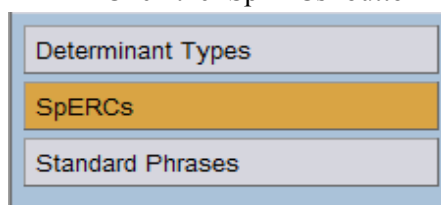
Then follow these steps:

- Open and log into CHESAR 3.3.

- Within CHESAR, click on the 'library management' button

Note: Please note a pre-requisite to run an exposure assessment in the CHESAR is to have a complete substance dataset



- Click the 'SpERCs' button in the sidebar



- Click the 'import' button in the main window, use the browse dialog to locate the upload file, then click on 'import'. This process should upload 4 SpERC files.

### 3.7.5 How to use the ECPA SpERCs in EUSES

The most recent version 2.1.2 of the European Union System for the Evaluation of Substances (EUSES) tool dating from 2012 is freely available at the webpage of the Joint Research Centre of the European Commission via the link:

http://crl-fcm.jrc.ec.europa.eu/our_activities/public-health/risk_assessment_of_Biocides/euses.

This example describes the input of the ECPA 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 ECPA 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 ECPA 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 ECPA 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:

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# 5   Appendices

*Appendix 1: Summary of changes between ECPA REACH-IN LET 2.0 and ECPA REACH-IN LET 3.0*

The ECPA REACH-IN Local Environment Tool (LET) v3.0 has been updated with the following changes:

- The Target RCR assumed for a 'Default' assessment has been reduced from 0.99 to 0.90

- The calculations for the 30 day and 180 day time weighted average concentrations in soil have been corrected to reflect the model description (see 3.6.2)

- The secondary poisoning assessment includes PECs for marine predator and marine top predator

- A background  PEC added at the local scale for the secondary poisoning assessment

- The safe dose calculation for secondary poisoning has been updated to account for the background PEC at the local scale

- Where the log $K_{OW}$ = 8 and 9, the $BMF_1$ updated to 10 and 3, respectively

- There is an option to specify measured BCF in fish and earthworms

- The Exposure Scenario tab has been restructured according to the format of the ECHA CSR template

- Automatic PNEC calculations improved. In some cases these were not updated correctly when input parameters were changed.

The effect of the above changes has been illustrated using four test substances with different physical-chemical, environmental fate and ecotoxicological properties which are summarised in Table A 1. Regional PECs for two exposure scenarios (one spray treatment and one granule treatment) were estimated using the ECETOC TRA v3.1. Each scenario was assumed to cover 100 tonnes in the EU and run using the ECPA SpERCs (ECPA SpERC 8d.1.v1 and ECPA SpERC 8d.2.v2). The resulting regional PECs were imported into the LET and substances were run as a 'Default' assessment with LET v2.0 (target RCR set to 0.9) and LET v3.0. The PNECs for sediment and soil were estimated by the LET using the equilibrium partitioning method.

**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).