Annex 2: Background document for all the proposed changes by workshop organising committee

1. Update of the QSAR models for BCF and Koc in EUSES

1.1. Current situation in EUSES

In the current implementation, EUSES offers the option of using QSARs for deriving a value for the input variables BCF and Koc. The Current QSAR for Koc (Sabljic) offers good performance[1] provided that the user has selected correctly the class that will be applied. Since the current implementation gives the user freedom to choose the chemical class of the substance, and depending on which one is chosen a different equation is applied, selecting erroneously the chemical class will affect significantly the final estimation of Koc, and thus the PEC calculations.

Regarding BCF, the current model in EUSES offers in general a reasonable estimation on the basis of Kow, which is in most cases conservative, but not always. The model was, however, developed for pesticides, hence the performance is worse for industrial chemicals.

In addition, no “structural domain check” is done on the calculations, so that if some fragments of a structure are not represented in the training sets of any of the models, the user will see no warning, but a higher error can be expected for the calculations.

1.2. Change proposed (what)

1.2.1. Option 1: Do nothing

Keeping the current implementation will be the most user familiar option for users, and allows calculating easily BCF and Koc. Obviously this does not require additional resources, but the chances of incurring in considerable errors without any warning remain there.

1.2.2. Option 2: Limit QSAR calculation domain

A possible refinement of the situation would be to give the option of applying the currently existing QSAR models, but having them available only for a limited set of substances:

- the QSAR for Koc would only be available for substances with logKow=<3 as the Koc is an information requirement for substances having log Kow>3 and
- the QSAR for BCF would only be available for substances with logKow=<4.5 as the BCF is needed for the PBT assessment for substances having log Kow>4.5.

For these cases, it is considered that having a (potentially) higher error for the calculations would not have a lot of impact as the potential for adsorption and bioaccumulation would usually be low (for ionisable substances for which the potential for adsorption will be high regardless of Kow a specific QSAR is proposed below). Since the user may not have the need to generate experimentally these parameters for REACH or BPR, keeping these QSARs would offer them an easy way of getting an input value for EUSES.

For the Koc, (for substances with logKow<=3) we propose two different calculations:

- For neutral organic chemicals, apply the equation for “predominantly hydrophobic chemicals” from the Sablijc model, which yields a conservatively high value:

$$Koc = \frac{1.26 \cdot Kow^{0.81}}{1000}$$

- For ionisable chemicals, it would be possible to apply the equations proposed by Franco and Trapp as explained in the RIVM report “Identification and preliminary analysis of update needs for EUSES[2]”. This would also require the user to provide a pKa value. The equations are:

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[1] Gerrit Schüürmann, Ralf-Uwe Ebert and Ralph Kühne *Environ. Sci. Technol.*, 2006, *40* (22), pp 7005–7011

[2] Available from https://echa.europa.eu/documents/10162/13630/echa_2014_253_euses_report_en.pdf/35a43ff6-4186-4c82-b1fd-8a7742cbfcdf

- For acids: $\mathrm{Koc_a} = \mathrm{Fn} \cdot 10^{0.54 \cdot \log(\mathrm{Kow})+1.11} + (1-\mathrm{Fn}) \cdot 10^{0.11 \cdot \log(\mathrm{Kow})+1.54}$

  where $\mathrm{Fn} = \dfrac{1}{1+10^{\gamma \cdot (\mathrm{pH}-\mathrm{pKa})}}$ and
  "γ" equals 1 for monovalent acids and -1 for bases
- For bases: $\mathrm{Koc_b} = 10^{0.31 \cdot \log(\mathrm{Dow})+2.78}$

  where logDow = Fn · Kow

This implementation would require little effort and ensure that for the most relevant substances the higher error associated with the current implementation does not become an issue.

1.2.3. Option 3: Expand the current functionalities making use of QSARs developed in other tools

The implementation of the changes suggested below would tackle the current issues with Koc and BCF calculations, and offer some extra features, while requiring the highest investment in terms of resources and time.

1.2.3.1. Addition of chemical input and descriptor calculating functionalities

In order to offer better calculation options for BCF and Koc, the first step would be to allow add entering chemical structures, which are used as the input for most of the current QSAR models using SMILES or a drawing user interface, as well as the ability to calculate the input values used by the QSAR models, and checking whether a structure is covered by their training sets.

A more pragmatic alternative would be connecting EUSES with a library of more updated QSAR models, implemented in a software platform offering these possibilities, such as EPISUITE, ChemProp or VEGA.

1.2.3.2. Improvement of adsorption desorption (Koc) models

The three possibilities suggested are:

- Keeping the current model (Sabljic), adding features allowing to select automatically the submodel for the right class, and checking that the target substance is covered by the training set of the model. These features are already implemented in ChemProp, so connecting EUSES to this software would implement this solution.
- Connecting EUSES with EPISUITE and offer the option of applying the MCI model from, which seems to offer a slightly better overall performance, although the "structural domain check" would be missing.
- Connecting EUSES with ChemProp, and use one of the models in this software. The most updated one in this platform, and reporting the best performance, is the one by Schuurmann et al (2006)[1]. It includes an automatic domain check. The model from Franco and Trapp (2011) is also available from this platform.

1.2.3.3. Improvement of bioconcentration factor (BCF) models

The following alternatives are suggested:

- Keeping the current model (Veith et al 1979), but implementing a "domain check" module to verify that a substance is well covered by the training set of this model.

  Log BCF (L/kg) = 0.85 x log Kow – 0.7 (if log Kow ≤ 6)
  and the modified Connell equation:
  Log BCF (L/kg) = - 0.2 log Kow2 + 2.74 log Kow - 4.72 (if log Kow > 6)
  The BCF for log KOW 1 and 10 are used when log Kow is < 1 and > 10, respectively.

  ChemProp has available this feature, and includes and additional refinement for the original Veith model.

- Using the Meylan model: this model accounts for some correction factors in addition to the logkow correlation, such as the presence of very long side chains or a phosphate ester functionality. It may be better suited for industrial chemicals. It is implemented in the EPISUITE package and also in VEGA and ChemProp. In the case of this last two platforms, it includes an automated domain check.
- Using the Arnot Gobas model: takes into account biotransformation of the molecule. Performs in general better than the Meylan Model, particularly for very hydrophobic chemicals. It is implemented in EPISUITE.
- Using the CAESAR model: it combines a model with several descriptors (not only logkow) and structural alerts, with the addition of an automated domain check. Performance is comparable to the Meylan model[3]. It is only implemented in the VEGA software.
- The model from Franco (2011) suggested by RIVM[2] (see also supporting information in the annex) could also be a good possibility for replacing the current QSAR, although it is not currently included in any software platform including automatic domain checks.

1.3. Why to propose such change

The koc models in EUSES offer good performance[4] (reported Q2 = 0.799, SE = 0,541), provided that the user has selected correctly the class that will be applied.

For instance, for a substance with logkow=3, the lowest logkoc calculated by the Koc equations is 3.9, and the highest 5.43 (1.54 log units of difference). The effect is more dramatic for very hydrophobic substances, so that for a substance with logkow = 7 there is a difference of more than 3.5 log units (9.1 - 12.67) between the different classes.

Regarding the BCF models, although the Veith model is in general conservative, that is not always the case. The magnitude of the error of a BFC calculation is related to whether the compound is inside the applicability domain of the model (parametric and structural) or not. This domain is quite small due to the fact that it was developed with very few chemicals.

Most of the compounds inside the applicability domain are within an error of 1 log unit, whereas around half of the compounds outside the applicability domain have an error > 1 log unit, and this error could be underestimation or overestimation.

- Option 1: “Doing nothing” will continue presenting this issues.
- Option 2: “Limiting the calculation domain” will reduce a bit the features of EUSES, but minimise the risk of high calculation errors for the cases which matter most.
- Option 3: “Expanding the current functionalities” is more resource intensive, but would reduce also the risk of calculations wrongly performed and improve the accuracy of the results.

1.4. Support for implementation

References

- Gerrit Schüürmann, Ralf-Uwe Ebert and Ralph Kühne Environ. Sci. Technol., 2006, 40 (22), pp 7005–7011
- https://www.umweltbundesamt.de/en/publikationen/comparative-analysis-of-estimated-measured-bcf-data
- Gissi et al. Environ Res;137:398-409

Software tools:

The following freely available tools already have implemented several models which could be used for the EUSES update:

- EPISUITE (current version 4.1). Support for the implementation and licensing issues need

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[3] Gissi et al. Environ Res;137:398-409

to be dealt with the US EPA, which could be administratively complicated.

- VEGA (current version 1.1.4). Support could be obtained from the Mario Negri Institute for Pharmacological Research (IRFMN) or Kode Chemoinfomatics, the company coding the software. Some modules already include an API which allows to call them from another software.
- ChemProp (current version 6.6). A user license is need for the use, even if it is free of charge. Support from the implementation of a docking with EUSES could be obtained from the Helmholtz Centre for Environmental Research - UFZ.

1.5. Priority level

1. Number (type of) of chemicals affected: All of the substances for which a Koc or BCF value is not available. All the chemical classes will be affected by options 2 and 3.
2. Maturity of the improvement: Option 1 is already implemented. Option 2 is well described and easy to document. Option 3 will require further discussions on the exact tools and models to be chosen.
3. Implementation in IT tools: Option 2 does not require a particularly complex IT implementation. Option 3 is, in contrast, more IT intensive, and potentially quite complex.
4. Regulatory considerations: Option 1 does not offer any improvement, while option 2 and particularly 3 would help better the users to meet their regulatory needs in a reliable manner.
5. Expected impact on exposure: Option 2 and 3 would increase the accuracy of exposure estimations, and reduce the risk of getting values which are wrong by a large margin.
6. New data requirement: pka would be necessary for some cases in option 2. SMILES would be necessary in option 3

Proposed overall assessment:

Option 1 does not offer any added advantage, apart from not requiring any effort.

Option 3 would improve the capabilities of EUSES, but requires further scientific and IT discussions, and could be cumbersome and expensive to implement.

We think that **option 2**, limiting the applicability of current QSARs, is the most cost efficient, addressing the problems linked with the potential lack of accuracy of the implemented models in certain situations, while requiring a quite light implementation.

1.6. Open question

- Which of the three proposed options is more effective in terms of resources/ impact?
- If Option 2 is chosen, is the proposed cut-off of logkow=<3 [resp 4.5] the most appropriate?
- If option 3 is chosen, which software platform should be connected to EUSES, and which models offered as an option?

Annex: additional information on RIVM proposal for updating the BCF QSAR

Many improved methods are available and discussed elsewhere (e.g. Environment UK 1999, Arnot et al., 2010) and additional consensus seeking may be needed to decide on the best overall approach. The choice for an updated model depends on the reliability of the model, the chemical domain that is covered by the model, and the appropriateness for risk assessment (explicit treatment of prediction uncertainty or degree of conservativeness).

The current approach in EUSES does not take biotransformation into account while the newer methods do. This is especially significant for strongly bioconcentrating/bioaccumulating chemicals (log Kow >5) where potential biotransformation can have a great impact on the predicted fish BCF and associated risks for human consumption. However, biotransformation in fish is not frequently available and may be either obtained via a fish BCF test or calculated possibly using QSAR models.

RIVM has proposed to replace the EUSES equations for bioaccumulation of neutral organic chemicals in the aquatic food chain with updated equations to estimate the bioconcentration factors (BCF) and biomagnification factors (BMF), based on e.g. Franco et al., 2011 or Rorije et al. 2011.

Rorije et al. (2011, section 2.2.2, (P)B score) used the REACH guidance R11 (ECHA, 2014, Appendix R11-1) as the basis for deriving an improved generic BCFmax estimate for the first trophic fish level, without biotransformation

$$\log BCF_{\max} = \frac{34.43}{2.93 \cdot (2 \cdot \pi)^{0.5}} \cdot e^{-0.5 \cdot \left(\frac{\log K_{ow} - 6.52}{2.93}\right)^{2}}$$

For input, both models (Franco et al., 2011; Rorije et al., 2011) require the same substance properties and environmental concentrations as the EUSES fish model (i.e. log Kow and the chemical’s freely dissolved concentration in water). The OSIRIS model (Franco et al., 2011) predicted considerable higher concentrations in fish than the EU TGD excel sheet. To take into account potential biotransformation, the biotransformation half-life in fish can be used in both models as well.

BCFmax is then subsequently corrected for biotransformation. The half-life due to metabolism is not standard input in EUSES.

The revised BCFs either based on Franco et al. (2011) and/or Rorije et al. (2011) can be used as input for calculating of the risk characterization ratios for secondary poisoning for birds and mammals (intermediate or top-predators).

In principle, all substances that undergo an assessment for secondary poisoning are affected due to the changes implemented, but on a general note, bioaccumulation is mostly of concern for substances with a log Kow value > 5. In addition, substances that undergo significant biotransformation will also be affected.

2. Overview of “release scenarios” and proposal to revisit the current approach for designing the release module

2.1. Introduction

A **Release scenario** is characterised by its release routes (to which compartment is the substance directly released) and possibly other factors, such as the number of days during which emission occurs or some specificity of the receiving environment. A number of different models exists (or will be developed) to estimate the local exposure in the different target compartments for those various release scenarios.

Currently a unique release scenario is supported by EUSES for REACH assessors. A number of release scenarios exist for biocides.

A biocidal product of a given PT may have different applications (scenarios) with different release scenarios i.e. with different emission pathways. For example wood preservatives may be applied at a sawmill as preventive treatment, or in situ on a house or on a fence, as preventive and/or curative treatment. For each of these applications a different set of conditions of use is assumed, leading to different amounts released, possibly via different routes. The releases from treatment of wood in the industrial plant (sawmill) will be to the STP while the treatment in-situ or service-life of treated wood (house, fence, bridge) will result in direct emissions to soil or water. Specific models for estimating the local exposure have been developed and integrated into the scenarios.

The following table lists the various possibilities that are (or intended to be) supported in EUSES for assessing local concentrations for various release scenarios.

- The compartments to which releases take place are differentiated for soil and water. Depending on the release scenario **one** receiving compartment within each release route may be selected.
- For a compartment receiving directly the releases (e.g. air, surface water, marine water), one or more models are (will be) available. Only **one** model is applicable for one assessment case.
- The release via one route to the receiving compartment, will impact on exposure in subsequent compartments. The exposure in a given compartment may be impacted by releases via several routes, which have then to be summed up. The existing models may already account for this, otherwise such summing need to be implemented.
- The last column indicates to which compartment the substance is released in the region (for SimpleBox, relevant under REACH). Note that in SimpleBox there is only one receiving surface water compartment.

Release route	Local direct release to	Local exposure concentration **based on the model** for receiving compartment	Local exposure in subsequent compartment impacted	Regional release to
Air	Air (kg/day)	Local concentration in air: release from industrial site	• Local agricultural soil • MvE (man via environment)	Air
		Local concentration in air: from application by spraying on a large surface (e.g. during spray application of mixtures on agricultural soil)	• MvE	Air
Soil	Agricultural soil (kg/ha.day)	Local concentration in agricultural soil	• Local concentration in water: Small static water (ditch): • Local concentration in sediments: Sediment (of the ditch): • Concentration in groundwater • MvE • Secondary poisoning (terrestrial predators)	Agricultura l Soil
	Non agricultural	Local concentration in non agricultural soil	• Concentration in groundwater	Non agricultural soil

	soil[5] (kg/day)			
Water	Biological STP (kg/day)	STP concentration (Based on SimpleTreat)	• Local concentration in agricultural soil after 30 days (for soil assessment) • Local concentration in agricultural soil after 180 days (for MvE, sec pois.) • Air • Freshwater surface water • Freshwater sediments • Marine water • Marine water sediments	waste water Note at the moment only 80% assumed via STP and 20% via surface water
	Surface water (kg/day)	Local concentration in water: flowing water	• Sediment • MvE • Secondary poisoning (predator)	Surface water
		Local concentration in water: static water (Pond)	• Sediment • MvE • Secondary poisoning (predator)	Surface water
		Local concentration in water: small static water surrounding agricultural field (ditch)	• Sediment • MvE • Secondary poisoning (predator)	Surface water
	Marine water	Local concentration in marine water Note: for generic scenarios the same amount could be assumed to be locally released to marine and surface water(flowing water)	• Marine Sediment • Secondary poisoning (predator) • Secondary poisoning (top predator)	Surface water Unless it duplicates the release to freshwater
		Local concentration in marine water (static: Oil platform)	• Marine Sediment • Secondary poisoning (predator) • Secondary poisoning (top predator)	Surface water
		Local concentration in marine water (Harbour scenario, semi static)	• Marine Sediment • Secondary poisoning (predator) • Secondary poisoning (top predator)	Surface water

The following table illustrate a few existing release scenarios:

Example of release scenario	**Direct release to**
"standard scenario"[6] used within REACH and sometimes for biocide	Air (water) STP Non agricultural soil for regional only (e.g. from ERC for outdoor uses)
Application of agrochemicals (pesticide/fertilizers)	Air (when spraying) Agricultural soil Surface water (small static water -ditch) (when spraying, via drift)
Application of construction chemicals to a building	Non agricultural soil
Leaching from building during service life	Non agricultural soil
Application of chemicals on a bridge	Surface water (static)
Leaching from treated bridge during service life	Surface water (static)

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[5] The "non agricultural soil" is a protection target not defined under REACH for local assessment. The release to soil from ERC for outdoor is to "non agricultural soil" but is used only for regional input.)

[6] This "standard release scenario" consists of a direct local release to a wastewater collection system and a release to air (from an industrial site). Indirect release to agricultural soil via the application of sewage treatment plant sludge and air deposition, as well as release to water and sediment from the effluent from the municipal biological STP are assumed. Local exposure to air, agricultural soil, STP, freshwater and freshwater sediments, marine water and marine sediments, as well as concentration in groundwater and in various food items used to assess secondary poisoning or exposure of man via the environment are calculated.

Storage of articles (e.g. treated wood) on soil	Non agricultural soil Surface water (static)
Swimming in lake	Surface water (static)

2.2. Why to re-consider the current approach for the implementation of the various biocides release scenarios

As described in the section above the approach for the estimation of local concentration based on release scenario is slightly different between REACH and biocides (a number of release scenario for biocide, a unique scenario for REACH). In the current version of the tool the two approaches are implemented in parallel. However, there is scope for synergy specifically for scenarios covering direct release, more consistency across regulatory areas and rationalisation of programming:

- Some of the release scenarios developed for biocides may be useful for assessments under REACH (for example some registrants have been requesting for scenarios of direct release to water for some outdoor uses). As a consequence the current separation between REACH and biocides scenarios should be made more flexible (e.g. also enabling contributing to the regional exposure assessment from those scenarios)
- The various ESDs for biocides (around 22 at the moment) have more or less similar release scenarios and only a few models exist to calculate a local concentrations in a given compartment. Often the values set for the model parameters (e.g. receiving water volume or soil volume) differ between the release scenarios. The equations for those scenarios are nevertheless not always described in the same way. For more consistency it may therefore be useful to have a clearly set model, with the possible option to modify a few parameters. More analysis of what is similar and what is the same is needed.
- Streamline the implementation of the various release scenarios with a limited number of models for estimating local exposure would not necessarily have an impact on the user interface and the ways of selecting the relevant scenario. However, it is proposed to more systematically distinguish between i) the release estimation and ii) the exposure estimates in the receiving compartment. In the current version of EUSES local exposure estimates are sometimes displayed within the release section. It is proposed that those should systematically be displayed in a consistent way within the exposure section.

In addition additional release scenarios such as direct releases to agricultural soil (topic 4) or releases from reservoirs (topic 5) will be added to the pool of available scenarios.

2.3. Priority level

The approach for developing EUSES with regard to the considerations above has to be further analysed during the pre-study expected to take place in early 2019. The streamlining of the implementation of the various release scenarios is seen as very important from the IT development perspective, but also to increase the consistency and rationalisation within and between the regulatory areas.

3. Release estimation module update

3.1. Current situation in EUSES

The latest EUSES version i.e. EUSES 2.1.2 (2012) is an update of EUSES 2.1 and contains in the release module for biocides the Emission Scenario Documents (ESDs) per product types which were prepared before 2010. For REACH the release module is still based on the use categories and default emission factors described in A-Tables and on the estimates for the fraction of the main source and the number of days for emissions from B-Tables of the TGD (EC, 2003). (EC, 2003).

3.2. Change proposed (why and what)

In the meanwhile many of the emission scenarios described in the ESDs have been updated based on decisions of the Environment Working Group (WG), the current EUSES version is therefore outdated and no longer usable. In addition some of the ESDs have been replaced by new versions. These changes are currently captured in the ESD calculation sheets per PT, available on the following ECHA webpage: https://echa.europa.eu/guidance-documents/guidance-on-biocides-legislation/emission-scenario-documents.

Therefore we propose to update the release module for biocides based on the existing ESD calculation sheets which reflect the latest status of emission estimations for biocides. Note that these calculation sheets are currently being implemented in a new EUSES version 2.2.0 in the frame of the “EUSES quick fix project”. This new EUSES version is planned to be released in Q4 2018.

The following updates described on a high level are already reflected in the ESD calculations sheets and need to be reflected also in EUSES:

- New sub-scenarios per PT developed after 2010 to be added to already existing emission scenarios
- Changed and newly agreed default values to be exchanged/added[7]
- New/revised ESDs prepared after 2010 needs to be added (e.g. for PT 13, PT 19 and PT 6)

At the time the EUSES update will be performed it is assumed that the EUSES quick fix is finalised and the new EUSES version 2.2.0 including an updated release module is available as basis for the EUSES update. Emission scenarios developed after the release of EUSES 2.2.0 however will need to be added in the release module in the frame of the EUSES update.

In addition, it is suggested to implement the approach proposed in the ECHA Guidance, Chapter R.16 for the default release estimation on tonnage basis. More specifically, default release factors associated to the Environmental Release Categories (ERCs) should be provided to be used as default input parameters, instead of release factors from A-Tables of the TGD (EC, 2003), to derive the environmental release rates in the updated release model. To select an appropriate ERC, the use description will also have to be adapted to be in line with the life cycle stages concept described in ECHA Guidance Chapter R12. In addition, instead of estimates for the fraction of the main source and the number of days for emissions from B-Tables of the TGD (EC, 2003) the following default parameters are proposed to be used in accordance with Guidance R16:

- Default number of release days based on life-cycle stages and tonnage per site as provided in the Table R.16-2 of the ECHA Guidance, Chapter R.16;
- Tonnage for uses at industrial sites (for both local and regional assessments): by default the annual use amount at a site is set equal to 100% of the tonnage for the use.
- Tonnage for widespread uses:
    - For local assessment: tonnage for the use (tonnes/year) × “tonnage for the use” used in the region x 5.5 10^{-6} year/day[8] ().
    - For regional assessment: it is set equal to 10% of the tonnage for the use.

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[7] Note that default values should remain modifiable if suitable justification/ data are available

[8] this constant takes into account the fraction of the regional tonnage used in a “standard town” and the number of days in the year which is always set to 365 for a widespread use

As in the current version of the model, the option to overwrite default release factors (e.g. to use release factors from Specific Environmental Release categories (SPERCs)), number of emission days and to use site-specific tonnages should be available in the updated version. If available, release rate could also be used directly in the model as input parameter.

The changes described above will have to be considered also in the context of the new implementation which may be proposed as initially described in topic 2, valid both for REACH and biocides.

3.3. Support for implementation

The sources of information to build the models supporting the proposed emission scenarios for biocides are listed below:

- ESD calculation sheets (see section 1.1) – prepared based on decisions of the Environment Working Group (WG) on scenarios/default values
- EUSES version 2.2.0, currently under preparation in the frame of the "EUSES quick fix" project

Release estimation according to R16 is already implemented in Chesar.

3.4. Priority level

For the implementation of new / modified ESD for biocides:

1. Number (type of) of chemicals affected:
    - Biocidal active substances
    - Substances of concern in biocidal products
    - Metabolites of biocidal active substances
    - Pre-cursors of in-situ generated biocidal active substances
2. Expected impact on exposure: PECs following direct release needs to be reflected in the fate and distribution part.
3. Maturity of the improvement (e.g. scientifically documented/ further research needed): the changes are well documented in (new) ESDs as well as in the Technical Agreements for Biocides (TAB).
4. Implementation in IT tools: the emission scenarios are implemented the ESD Excel sheets as well as in the future EUSES version 2.2.0.
5. Regulatory considerations: no impact on the regulation since the proposed changes are already agreed by the relevant regulatory body (i.e. the BPC Environment WG).
6. New data requirement: no new data needed.

<u>Suggested priority:</u> Ready and high importance since the proposed change is mandatory to make EUSES usable for biocides.

For adaptation of default local tonnage and default local release factors according to R16

1. Number (type of) of chemicals affected: All substances for which the release rate is estimated by default
2. Expected impact on exposure: Possibly high impact on the default release estimation. The proposed change is fundamental improvement of low tier risk assessment which would be based on conservative input parameters when no risk is identified. This would result in higher conservatism of the assessment and give higher confidence to the positive, i.e. 'no risk identified', outcome of it.
3. Maturity of the improvement: fully described in ECHA Guidance, Chapter R.16
4. Implementation in IT tools: implemented in CHESAR
5. Regulatory considerations: in line with endorsed default approach for the release estimation for the CSA under REACH Regulation.
6. New data requirement: no new data needed.

Suggested priority: Ready/ high importance as this should support the default release assessment under REACH

3.5. References

EC, 20013. Technical Guidance Document on Risk Assessment (TGD) in support of Commission Directive 93/67/EEC, Commission Regulation (EC) No 1488/94 on Risk Assessment for Existing substances, Directive 98/8/EC of the European Parliament and of the Council concerning the placing of biocidal products on the market).

ECHA Guidance on information requirements and Chemical Safety Assessment, Chapter R.16: Environmental exposure assessment (Version 3.0, February 2016)

ECHA Guidance on information requirements and Chemical Safety Assessment, Chapter R12: Use description

Technical agreements for biocides (TAB) v.1.3: https://echa.europa.eu/documents/10162/20733977/technical_agreements_for_biocides_en.pdf/4280fdc4-dfb0-405e-898e-70f3cdf62ce2

4. New release scenario: direct releases to agricultural soil

4.1. Current situation in EUSES

There is no release scenario and local exposure estimation for direct releases to agricultural soil (for example application of fertilizers, plant protection products[9]) with the exception of the emission scenario for manure application (PT 18: Insecticides and PT3: Veterinary hygiene).

Exposure of agricultural soil is nevertheless estimated in the current version of EUSES.

- Local exposure resulting from indirect emission to agricultural soil via application of biological STP sludge over 10 years and via deposition from air emissions. The concentration in agricultural soil 30 days after the last application is used for PECsoil. The concentrations in grassland and agricultural soil 180 days after the last application are used as input to the models calculating exposure in various food items for man via the environment (MvE) exposure and for secondary poisoning. The current models do not account for run off to surface water for PECwater calculation; however, losses of the chemical in soil due to mechanisms such as volatilisation, leaching and degradation are taken into account.
- Direct releases to agricultural soil can be considered at the regional scale.

4.2. Change proposed (what and why)

We propose to include a release scenario covering direct releases to agricultural soil. Direct release to water (via drift) and to air may also occur for example during spray application.

If not implemented in EUSES, assessors who need to cover direct releases to agricultural soil need to use other tools available on the market to estimate exposure. This has two main disadvantages:

- No harmonisation across registrants as several tools are now being developed, leading possibly to a lack of trust from the authorities
- For a substance used in several applications (as such or in mixture) several models will need to be used. This makes the estimation of the regional exposure more complicated.

An additional benefit is that the link to Chesar is ensured from EUSES. Therefore for registrants using Chesar and needing such scenarios, they would not have to manually report the outcome of his assessment made with a specific tool in Chesar.

This proposal is derived from the ECPA LET tool because of the availability of a complete description of the model equations reported in the source documents.

The “default” scenario in the LET tool[10]considers:

- Only one application per year (frequency of application and intervals between applications not accounted for)
- A number of assumptions (not changeable by the user) for the estimation of environmental concentration; for example, no removal of substance from crop interception, worst case value for run off from soil to surface water, etc.

However, as both ECPA LET tool (see ref [1]) and FEE tool (see ref [3]) could be used for the “direct releases to agricultural soil” scenario, discussion with the tool owners is foreseen after the workshop to identify the best approach to be implemented in EUSES. This approach could be a refined combination of the scenarios available in both ECPA and FEE considering the necessary balance between flexibility and easiness of use/implementation of the new release scenario.

Furthermore it should be also highlighted that, whereas direct emission to air is considered in the SPERCs covering application of co-formulants of PPP (spray application), there is no estimation, in the LET tool, of the local air concentration following these emissions. Consequently

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[9] Co formulants of PPP are to be registered and assessed under REACH

[10] More options will remain available in the LET tool for “refined scenarios”.

a way to estimate concentration in air (for exposition of man via the environment mainly) is to be integrated.

4.2.1. Release scenario

It is assumed that the starting point for this scenario is direct release to:

- Agricultural soil via an application rate (kg/ha.day) assuming only one application per year (therefore tonnage used over the year should be used if several application would be assume din reality)
- Static water (ditch) possibly via drift for spray application
- Air for spray application

4.2.2. Soil compartment

For estimating the local concentration in agricultural soil the ECPA LET default scenario could be slightly modified to take into consideration the accumulation over years like in the "standard release" scenario in EUSES[11]. In ECPA LET, the soil compartment is represented by 1 hectare of agricultural soil homogenously mixed over 0.05 m[12]. Soil loading comes from direct releases to soil after application. The PEC in soil is calculated as a 30-day time-weighted average following the application event[13] and includes losses through biodegradation, leaching and volatilisation. This time averaging approach is in accordance with the ECHA R.16 guidance; the groundwater concentrations and local soil concentration used for secondary poisoning is averaged over 180 days (in line with R16 guidance).

4.2.3. Water compartment

The LET tool for estimating the local concentration in water and sediments is based on the STEP 2 of FOCUS [Ref 3].

A water body surrounding the 1 hectare of soil is the receiving water compartment. It has the following dimensions: 30 cm water depth overlying 5 cm of sediment; sediment is assumed to have 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), which means 1000 m^2 waterbody with a volume of 3 x 10^5 litres; the water is considered as "static".

The loading to the surface water is coming from the following sources:

- Drift, which is considered as direct release to water (to be included in the release factor to water)
- Run off (drainage), which happens in this scenario 4 days after the soil treatment;

The fraction of run off is expressed as a percentage of the soil residue moved to the waterbody, assumed to be 5 % (worst case estimated by ECPA from observations within different regions and periods), meaning that 5% of the amount present in the soil at the moment of the run off goes to the whole water compartment (water + sediments)[14].

The daily concentration in water and sediments is estimated up to the day after the run off event (i.e. up to 5 days after application) taking into account biodegradation (in water and in sediments). As the receiving water body is a "static" water with limited dimension, ignoring biodegradation may lead to a very large over estimation of exposure. The maximum daily

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[11] Please note that ECPA tool does not consider accumulation over 10 years of application, while FEE tool does.

[12] Note that there is a difference between top 5 cm used in ECPA LET tool (standard for PPP assessments) and standard depth of soil compartment under REACH (20 cm for agricultural soil). While the former can be used for calculation of peak concentrations within a growing season, the latter is regarded more relevant for accumulation over different growing seasons. In the ECPA LET tool it is possible to take account of soil incorporation (ploughing) as refinement option, in this case a mixing depth of 20 cm is also assumed.

[13] See also proposal for providing an initial PEC soil (topic 12)

[14] An alternative estimate of run off is provided in FEE tool, derived from Simplebox-based equation

concentration over those 5 days is set as local concentration in water[15]. The same applies for setting the exposure in the sediment compartment.

The sediments are considered as a separate compartment receiving a fraction of the loading (via drift and run off) to the whole water compartment (surface water and sediment). Such fractions depend on the day of exposure and on the type of loading (drift or run off).

Local PECs are calculated summing up the PECregionalwater to the local concentration, for both water and sediments. In the LET tool the local concentrations in marine compartment can be obtained (although generally not relevant for this scenario) dividing freshwater local concentrations by a factor of 10

4.2.4. Secondary poisoning

The secondary poisoning (freshwater / marine water (top)predators, terrestrial predators) could be calculated as currently implemented in EUSES with the following difference proposed in the LET tool: the local PEC used for the water compartment is not averaged over the year as done in the standard model, instead a 21-day average concentration is used for assessment of secondary poisoning. Indeed as the assumption for the model is one yearly application, averaging the exposure over the year would lead to a potentially high underestimation of exposure for predators.

4.2.5. Exposure of man via the environment

The exposure of Man via environment is not considered in the “default” scenario in the LET tool described above.

- There is a need to define the air concentration possibly on the basis of the by-standers model mentioned in ECPA guidance for spray application (adaptation to be defined).
- For exposure of man via environment via the oral route the model already available in EUSES can be used for the estimation of the concentrations in the food items

4.2.6. Regional concentration

No changes are foreseen in SimpleBox. The regional releases should be to air, agricultural soil and surface water.

4.3. Support for implementation

The sources of information to build the models supporting the proposed scenario are listed below:

- Sludge application currently implemented in EUSES; while this needs to be completed (e.g. with run off contribution to surface water), it might constitute a good starting point in terms of how to take into consideration application rate expressed as kg/ha to agricultural soil.
- Manure application for PT 18 described in the related ESD.
- ECPA LET tool [Ref 1] developed by the European Crop Protection Association (ECPA) to cover direct releases to agricultural soil of co-formulants in plant protection products. It is based on a (simplified) version of FOCUS. Default assessment is available as well as refinement options. ECPA LET enables the calculation of concentrations in surface water and sediments due to air drift or run off; it does not include any module for calculation of local air concentrations.
- USES [Ref 2] model developed by RIVM, which includes a module to estimate local concentrations (soil, water, sediment and air) due to agricultural application of chemicals such as pesticides. It takes into account different mechanisms and exchange between compartments, and subsequent calculation of concentrations (in water, sediment, soil, air).
- FOCUS[Ref 3] programme developed under pesticides regulation

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[15] Note that different views exist on whether this is an adequate choice or whether such concentration should be considered as a “PEC intermittent” and that the PEC should be calculated as e.g. the 30 days time weighted average concentration.

- FEE tool [Ref 4] developed by Fertilizers Europe to cover direct application of substances in fertilizer products on agricultural soil. Conceptually similar to the ECPA tool (e.g. it contains a default conservative scenario and several refinement options, based on simplified FOCUS), it includes properties of predefined ingredients (inorganics).

4.4. Priority level

Criteria for priority evaluation:

1. Number (type of) of chemicals affected: substances present in specific products (such as co-formulants in plant protection products, substances in fertilizers); the number of substances affected by the change is limited.
2. Maturity of the improvement (e.g. scientifically documented/ further research needed): the change is well documented in several publications and, as such, implemented in several tools. Nevertheless there is no opinion of the authorities on their relevance. Therefore an analysis is needed for the identification of the best approach.
3. Implementation in IT tools: the agricultural scenario is implemented in several tools like USES (precursor of EUSES), FEE tool (Fertilizers Europe), LET (ECPA). Moreover, FOCUS is the framework of tools used for approval of active substances in pesticides.
4. Regulatory considerations: no impact on the regulation (the improvement fills a gap in exposure estimation under REACH). External tools such FEE and LET (the latter used in this proposal) already mentioned in R.16 guidance.
5. Expected impact on exposure and/or alternative solutions available: The scenario would be a new scenario in EUSES. Alternative models do exist (FEE and LET tool).
6. New data requirement: no new data needed. The exposure is run with the same substance specific parameter EUSES currently uses for exposure assessment.

<u>Suggested priority</u>: (nearly) ready, medium importance.

Medium importance since the proposed change, while filling a gap, concerns a relatively small number of substances. The proposal is already implemented in other tools but **decisions are to be taken for deciding on the options to implement in EUSES. It is suggested to discuss those details specifically with the sectors concerned after the workshop.**

4.5. Open questions

The following differences should be noted between the proposal made here (from the ECPA LET) and with the existing model of STP sludge application in EUSES:

- The LET tool does not take accumulation of substance in the soil over the years into account;
- The LET tool does consider the run off to a surface water and calculate PECs for water and sediment in the receiving water body (ditch surrounding the agricultural field)

The following options may be considered to align the models (further discussion needed):

- Implement a solution in EUSES for the estimation of the exposure to agricultural soil on the basis of the LET tool but taking into account accumulation over the years as currently done for sludge application
- Adapt the current model for sludge application from STP to also account for release to water/sediments via run off of agricultural soil. Note that such implementation would lead to 2 possible values for the PECwater: the one obtained in the surface water due to release from the STP and the one in the static freshwater (the ditch) from the run off of soil. The higher concentration may be different depending on the properties of the substance (in particular absorption potential). The maximum of these 2 values may be selected as a PEC

In addition as explained above the concentration in sediment is not calculated on the basis of the partitioning between water and suspended particles, as done in the other models implemented in EUSES (and as described in Guidance R16). A fraction of the amount release to water is directly transferred to sediments. It would probably need to be analysed what the differences in the two models are and whether alignment would be needed

4.6. References

[1] "*ECPA Guidance on REACH Chemical Safety Assessment for Co-Formulants Used in Crop Protection Products*", The REACH-IN Project, 19 March 2015. Available at: http://www.ecpa.eu/industry-resources/reach-registration-evaluation-authorisation-and-restriction-chemicals

[2] USES. Background document available at: http://www.rivm.nl/bibliotheek/rapporten/601450012.pdf. Application of pesticides see section P29

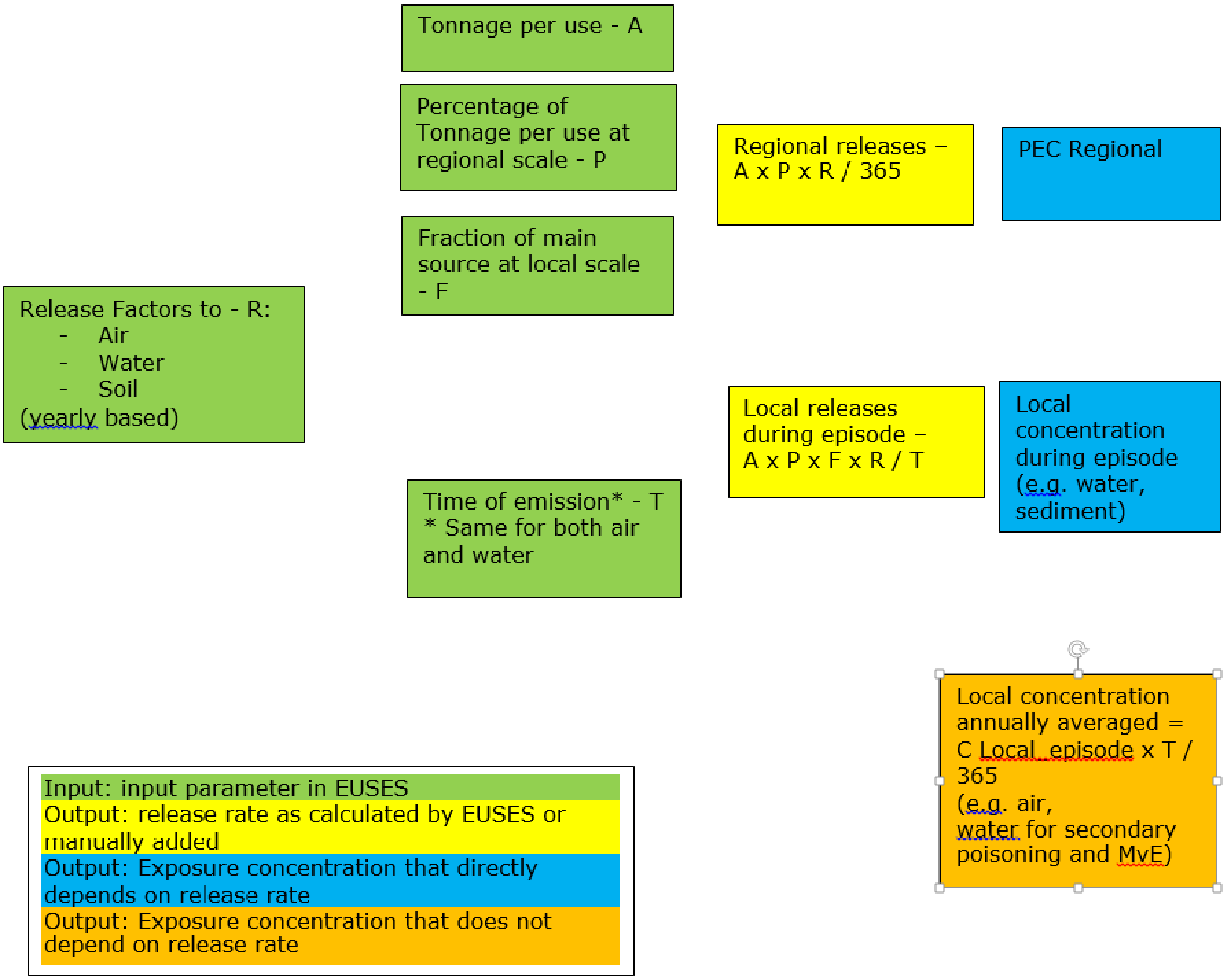
[3] FOCUS (2014). FOrum for Co-ordination of pesticide fate models and their USe, in the framework of the EU Directive 91/414/EEC. Website http://focus.jrc.ec.europa.eu/

[4] Fertilizer Europe (FEE tool) Available at: http://www.reachfertilizers.com/#fee

5. New release scenario: releases from "reservoirs" (taking account of temporal release patterns)

5.1. Current situation in EUSES

The flowchart below exemplifies how the current version of EUSES calculates amounts, release rates and correspondent exposure concentrations at different scales and timeframes when a tonnage based approach is used to estimate releases. Please, be aware that the flowchart is not complete in terms of calculation (continental releases not reported, as well as all uses contributions for regional PECs, etc.); it rather exemplifies in a simple way the main inputs and corresponding outputs.



What is important to notice is that in the current version, EUSES assumes that the releases to air and to water happen over the same period of time (T above).

5.2. Change proposed (why and what)

The current standard release scenario is suitable for most of the cases, but fails when the time of emission significantly differs for air and water release route; it might happen for example in the following cases

- When wet scrubbers are used and the content discharged over few days into water
- For baths (e.g. such used for metal surface treatment), when the daily losses are comparatively lower than the daily releases to water during bath exchange operations
- When the releases to water comes from cleaning operations only, but these operations are performed not every working day (for example few days/month)

Currently only few SPERCs are covering such scenario (e.g. ACEA SPERCs). However, the scenario potentially applies to many industrial uses where there is not continuous release to water over the working days.

For example, setting the time of emission equal to working days (e.g. 300 days/year) when the releases to water take place only few days during the year (e.g. 30 days/year, like when emptying batches or reservoirs) means, with the current EUSES, underestimate 10 times the emissions to water during the day of release, which means underestimate also 10 times the local PECs water and sediments.

In those cases even if the local releases during the episode are overwritten for air and water, the local concentration annually averaged would be wrong for one of the two routes.

Here below we describe how the new "reservoir scenario" should work.

The user, once selecting the "reservoir scenario", is invited to provide 2 different times of emission:

- Time of emission to air
- Time of emission to water

The 2 different times of emission are used (see flowchart above) to calculate:

- Local release rates (to air and to water) during episode
- Local concentration annually averaged for air and water compartment

Local PECs will then be calculated as currently done in EUSES.

If not implemented, assessors who need to cover the "reservoir scenario" would have to run EUSES twice and take some result from one and some from the other simulation; this would be inefficient and prone to errors.

5.3. Support for implementation

No particular supporting information are available for the proposed change.

5.4. Priority level

Criteria for priority evaluation:

1. Number (type of) of chemicals affected: the proposed change is scenario specific and not substance specific; however it is expected to cover limited number of cases.
2. Expected impact on exposure and/or alternative solutions available: when relevant, the new scenario might have an important impact on exposure concentration in water, sediment and soil (via sludge) compartments. Alternative models does not exist to cover this scenario.
3. Maturity of the improvement (e.g. scientifically documented/ further research needed): the change does not require scientific discussion and can be easily implemented in EUSES.
4. Implementation in IT tools: there are no other IT tools that implement the change proposed. EUSES would be the first.
5. Regulatory considerations: no impact on the regulation (the improvement fills a gap in release estimation under REACH). No need to guidance update as well.
   New data requirement: no new data needed. The exposure is run with the same substance specific parameter EUSES currently uses for exposure assessment.

<u>Suggested priority:</u> Ready, Low/Medium importance

The proposed change fills a gap and complete the possibilities for release estimation cases covered by EUSES; the change is easy to implement.

6. Update of SimpleTreat

6.1. Current situation in EUSES

In the latest EUSES version i.e. EUSES 2.1.2 (2012) SimpleTreat 3.1 is implemented, estimating chemical emission from sewage treatment plants.

6.2. Change proposed (why and what)

A new version of SimpleTreat, i.e. version 4.0 is available which takes up recent scientific insights with respect to the behaviour of the chemical in domestic sewage and activated sludge, which is proposed to replace the current version SimpleTreat 3.1. The model structure has not changed with respect to SimpleTreat 3.1. Version 4.0 is a no-equilibrium, steady-state multimedia model of the fate of a chemical. In SimpleTreat 4.0 new equations for sorption of organic acids and bases are formulated (as described in topic 1). Furthermore, default parameters defining the operation mode of a sewage treatment plants (STP) have changed according to the technological development in the EU the last two decades (for details on the differences compared to the version 3.1 see https://www.umweltbundesamt.de/sites/default/files/medien/378/publikationen/texte_13_2015_application_of_simple_treat_4.0.pdf).

With regard to the operation mode of STPs, an impact assessment was performed for biocides looking at revised default values proposed for BOD load, the sludge loading rate (SLR) and the suspended solids concentration in effluent (Css). Details are provided in the annex of this document. As a consequence we suggest to replace SimpleTreat 3.1 with SimpleTreat 4.0 with the exception that the default value for Css should remain 30 mg/L as it was in 3.1 instead of 7.5 mg/L as proposed in SimpleTreat 4.0. Indeed, data from the Netherlands on suspended solids concentration show a strong, declining trend over the years resulting in a revised value of 7.5 mg/L in SimpleTreat 4.0, reflecting the Dutch situation. In the absence of additional information in other countries however it was decided for biocides to keep the old value of 30 mg/L. Note that EUSES should keep the flexibility to overwrite default values when justification to do so exist.

6.3. Support for implementation

The sources of information to build the models supporting the proposed scenarios are listed below:

- Alone standing IT tool “SimpleTreat 4.0”
- EUSES version 2.2.0, currently under preparation in the frame of the “EUSES quick fix” project

At the time the EUSES update will be performed it is assumed that the EUSES quick fix is finalised and the new EUSES version 2.2.0. including SimpleTreat 4.0 is available.

6.4. Priority level

1. Chemicals affected: all substances are affected.
2. Expected impact on exposure: The current tool to assess the degradation/distribution in the STP will be exchanged.
3. Maturity of the improvement (e.g. scientifically documented/ further research needed): Well documented in the SimpleTreat manual and by the impact assessment performed for biocides.
4. Implementation in IT tools: SimpleTreat 4.0 is available as standalone tool.
5. Regulatory considerations: no impact on the regulation.
6. New data requirement: no new data needed. The exposure is run with the same substance specific parameter EUSES currently uses for the STP assessment.

Suggested priority: Ready/high importance

The proposed change is already implemented in Simpletreat 4.0 and provides an update of the current distribution model in the STP (already agreed for biocides).

6.5. Open questions

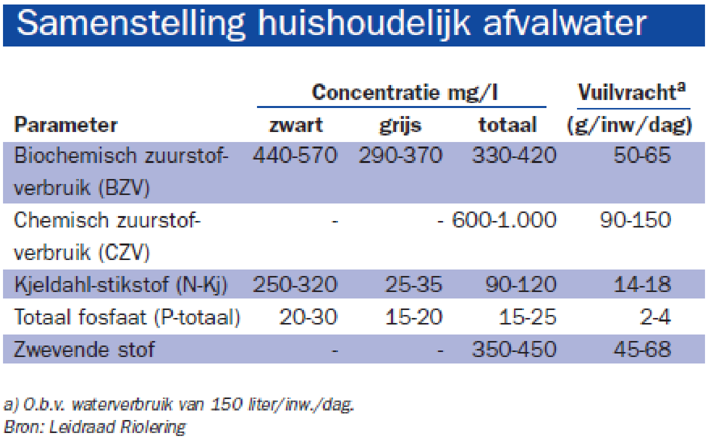
- Should the input parameters for SimpleTreat be handled in a flexible way so that different default values can be introduced (e.g. differently agreed SLR for biocides)
- Should SimpleTreat industrial also implemented?

Annex: Detailed proposals for changes of input parameters in SimpleTreat

In the following the changed parameters in SimpleTreat 4.0 compared to SimpleTreat 3.1 are briefly listed:

BOD in raw sewage

In SimpleTreat 3.1 the value of 54 g/person/d is used as default to define the BOD concentration in raw sewage entering the system at a rate of 200 L/person/d. This implies that the concentration in raw sewage is equal to 270 mg O2/L. This value is based on Van Haute (1975, see page 31) and Koot (1974, page 36).
In SimpleTreat 4.0 the default BOD input was set to 60 g/person/d which is equivalent to 300 mg O2/L for an unaltered sewage flow rate. For biocides, this value was agreed to be used. This value goes back to work of Imhoff and Imhoff (1985) and later work of Doorn and Liles (1999) came to the same result. This value is confirmed in European Urban Waste Water Treatment Directive (91/271/EEC): ‘1 p.e. (population equivalent)’ means the organic biodegradable load having a five-day biochemical oxygen demand (BOD5) of 60 g of oxygen per day, in IPCC (2006) and in UNEP (2016). Relatively recent numbers from The Netherlands point towards and even higher BOD content (see Figure 1) (Stichting RIONED, 2009). Until 2016 German municipal STPs have been planned according to the technical rule ATV-DVWK-A 131E (2000), which assumes a BOD of 60 g/person/d.


Samenstelling huishoudelijk afvalwater

	Concentratie mg/l			Vuilvracht[a]
Parameter	zwart	grijs	totaal	(g/inw/dag)
Biochemisch zuurstof-verbruik (BZV)	440-570	290-370	330-420	50-65
Chemisch zuurstof-verbruik (CZV)	-	-	600-1.000	90-150
Kjeldahl-stikstof (N-Kj)	250-320	25-35	90-120	14-18
Totaal fosfaat (P-totaal)	20-30	15-20	15-25	2-4
Zwevende stof	-	-	350-450	45-68

a) O.b.v. waterverbruik van 150 liter/inw./dag.
Bron: Leidraad Riolering

Figure 1: BOD (first row) in Dutch municipal STP’s (RIONED, 2009).
Translation: Title: Composition of domestic wastewater.
Biochemisch zuurstofverbruik (BZV) = biological oxygen demand (BOD).
Column 2, 3, 4 are BOD concentrations in mg/L; zwart = black, grijs = grey, totaal = total.
The last column 'Vuilvracht' = sewage load, is expressed in g BOD/inh/day, on the basis of a water use of 150 L/inh/day.

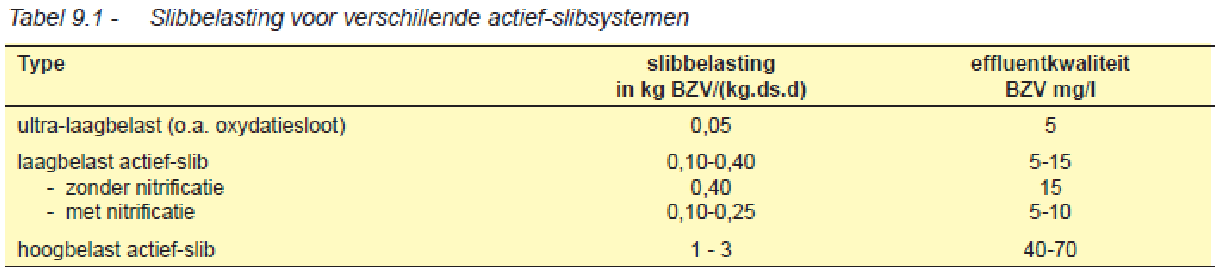
Sludge loading rate (SLR)

The default has been reduced to 0.1 kg BOD/kg MLSS/d as it is assumed that the average STP receives less BOD because the number of STPs in the EU has increased significantly the last two decades. For biocides, this value was agreed to be used.

Van Haute (1975, see page 157) shows a graph indicating empirical BOD reduction efficiencies versus the SLR. The range between 0.1 and 0.2 g BOD/ kg MLSS/d (MLSS is the biomass concentration in the aeration tank) typically represents modern STPs with a low SLR and a BOD removal rate of 90%. Also by Koot (1974, p 167) this relationship is given, indicating again that the SLR range of 0.4 and 0.05 g BOD/ kg MLSS/d represents a low sludge loading rate of modern STPs with an intermediate range of 0.1 and 0.2 g BOD/ kg MLSS/d.

SimpleTreat 3.1 applied a default value of 0.15 kg BOD/kg MLSS/d (MLSS is the biomass concentration in the aeration tank) for the SLR, also known as food to mass ratio (F/M).

In SimpleTreat 4.0 the default has been reduced to 0.1 kg BOD/kg MLSS/d as it is assumed that the average STP receives less BOD because the number of STPs in the EU has increased significantly the last two decades. Dutch data suggest that both the old value, as well as the revised default value for SLR are encountered in modern STPs and that both values fall within the range of STPs that support nitrification (see Figure 2) (TU Delft, 2008). According to Gujer (2006) the sludge loading rate for STPs supporting nitrification and denitrification, which is state of the art in Germany, ranges from 0.05 kg BOD/kg MLSS/d to 0.15 depending on the number of connected population equivalents and surplus sludge production.



Tabel 9.1 - Slibbelasting voor verschillende actief-slibsystemen

Type	slibbelasting in kg BZV/(kg.ds.d)	effluentkwaliteit BZV mg/l
ultra-laagbelast (o.a. oxydatiesloot)	0,05	5
laagbelast actief-slib	0,10-0,40	5-15
- zonder nitrificatie	0,40	15
- met nitrificatie	0,10-0,25	5-10
hoogbelast actief-slib	1 - 3	40-70

Figure 2: Sludge loading rates for Dutch STP's according to TU Delft (2008).
Translation. Table header: Sludge load for different activated sludge systems.
Column1. Types: ultra low load (oxidation ditch); low load activated sludge (without nitrification and with nitrification), high load activated sludge.
Column 2. sludge loading rate (SLR) in kg BOD/ kg_{dw} / d.
Column 3. Effluent quality (mg BOD/L). Not used in this comparison.

In SimpleTreat the sludge loading rate is one determining parameter for the hydraulic retention time (HRT) in the aerator. The longer the retention time of the wastewater in the aerator is, the higher is the rate of degradation and adsorption. According to Gujer (2006) typical hydraulic retention times in the aerator in modern STPs are 10 h (page 299). Table 1 summarizes the resulting hydraulic retention times in the aerator in SimpleTreat 4.0 for the two options of BOD and SLR, respectively, for an STP with primary sedimentation:

Table 1: Hydraulic retention times in the aerator (calculated with SimpleTreat 4.0) determined by the discussed parameters SLR and BOD

BOD [g/person/d]	SLR [kg BOD/kg MLSS/d]	HRT in aerator [h]
54	0.15	6.9
54	0.1	10.3
60	0.15	7.7
60	0.1	11.5

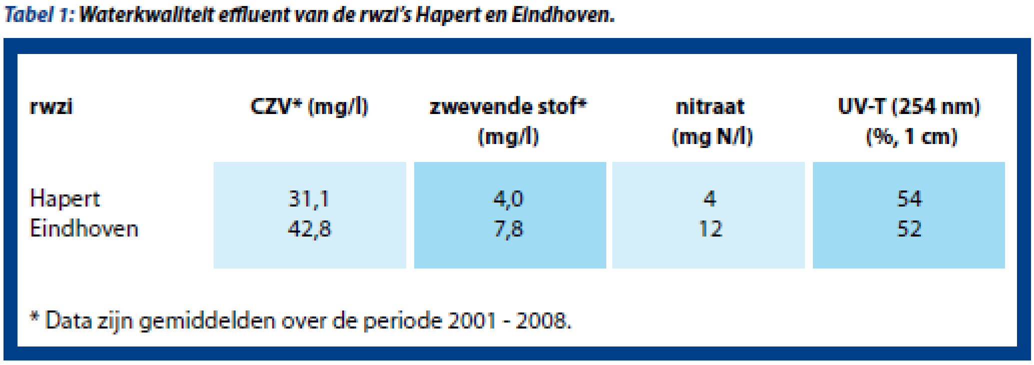
The HRT in the aerator derived from the SLR 0.15 kg BOD/kg MLSS/d is below the typical HRT of 10 h stated by Gujer (2006), whereas the HRT derived from the SLR of 0.1 kg BOD/kg MLSS/d are slightly above the 10 year old handbook value.

The downwardly revised default value for the SLR is plausible, as the total treatment capacity across the EU has increased significantly since the release of SimpleTreat v. 3.1. However, the available data vary considerably and do not point into a specific direction. The separate numerical impact analysis shows insignificant impact for not degrading substances and significant impact for readily biodegradable substances.

Suspended solids concentration of effluent (Css)

In SimpleTreat 3.1 a suspended solids concentration of 30 mg/l dry matter in effluent is assumed. For a conventional activated sludge treatment of municipal wastewater Van Haute (1975, see page 62) a concentration of 25 – 30 mg/l is mentioned. This value is also given by Koot (1974, page 174) for a moderately loaded activated sludge system although in graph this source also shows that for a significant share of STPs the concentration is between 5 and 15 mg/L.

Franco et al. (2013) states that operational conditions may have changed, as a result of evolving technologies and more stringent legal requirements for the effluent quality established by the EU Urban Wastewater Treatment Directive (91/271/EEC). The authors submitted SimpleTreat 3.1 to a probabilistic test in which several defaults parameters had been varied, among which the concentration of suspended solids in effluent. They concluded that the removal of total suspended solids over the last 2 decades improved. The probability density function for suspended solids in effluent was fitted to a representative set of monitoring data, including measurements from the UKWIR Chemical Investigation Programme for 58 activated sludge STPs (Gardner et al. 2012). A medium concentration of 8 mg/L was found to better reflect the STP emissions in the EU today. Additionally, Dutch data was found from overview studies, suggesting a range of 3 – 9 mg/L (see Figure 3 and Figure 4) (De Jonge et al. 2010, Van den Boomen & Kampf, 2012). The most accurate data for the Netherlands are shown in Table 2 below. Concentrations of suspended matter in STP effluent are collected and presented yearly by Statistics Netherlands (CBS, the Dutch national statistics institute (CBS, 2016). The data presented are average values for the whole country, although more detailed data are available. To illustrate the variability, the average value for 2014 is 7.1 ± 1.7 mg/L for 11 provinces in the Netherlands. The data clearly show a strong, declining trend over the years and underpin that the proposed value of 7.5 mg/L is a valid value for the Dutch situation.



Tabel 1: Waterkwaliteit effluent van de rwzi's Hapert en Eindhoven.

rwzi	CZV* (mg/l)	zwevende stof* (mg/l)	nitraat (mg N/l)	UV-T (254 nm) (%, 1 cm)
Hapert	31,1	4,0	4	54
Eindhoven	42,8	7,8	12	52

* Data zijn gemiddelden over de periode 2001 - 2008.

Figure 3: C$_{\text{suspended solids}}$ for two STP's in The Netherlands (De Jonge et al. 2010). Translation. Second column: 'zwevende stof' = concentration suspended solids (mg/L). Subscript states: data are averages over the period 2001-2008.

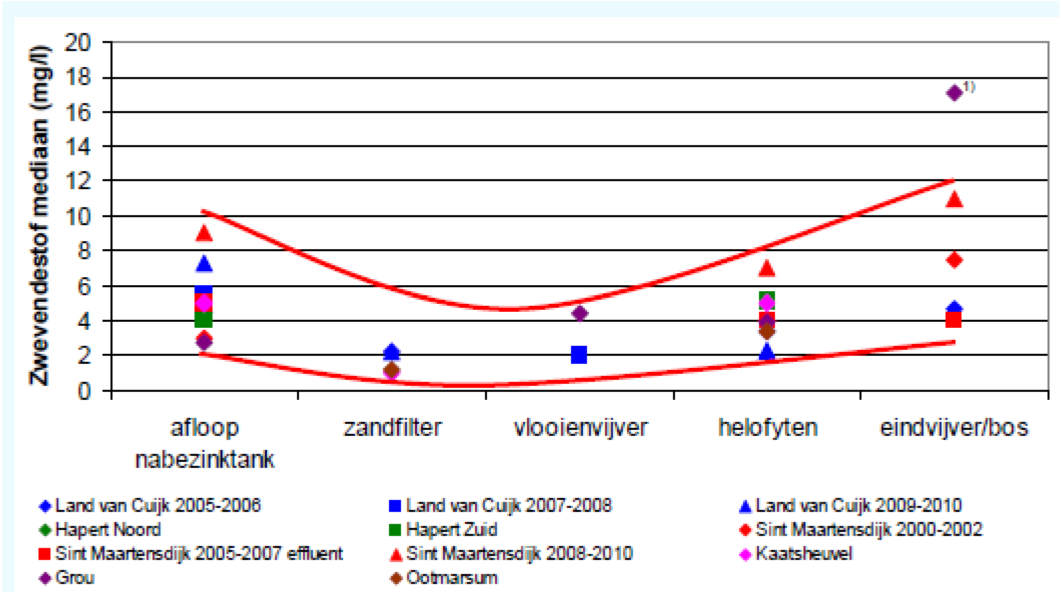


Figure 4: C$_{\text{suspended solids}}$ for four STP's in The Netherlands (Van den Boomen & Kampf, 2012). Translation. Y-axis shows Concentration in suspended solids (mg/L). X-axis shows five different wastewater-treatment systems, of which only the leftmost system on the axis represents STPs.
afloop nabezinktank = run out from settler
zandfilter = sand filter
vlooienvijver = pond with water fleas
helofyten = helophyte system
eindvijver/bos = 'end pond'/wood.

Table 2. Concentration of suspended matter in STP effluent. Average values for the Netherlands 1981-2014^{a}.

Year	C_{ss} (average for NL) [mg/L]
1981	47
1985	37
1990	28
1991	23
1992	19
1993	17
1994	19
1995	18
1996	20
1997	19
1998	27
1999	13
2000	21
2001	22
2002	18
2003	11
2004	11
2005	10
2006	11
2007	10
2008	9
2009	10
2010	10
2011	8
2012	8
2013	8
2014	7

[a]Source: CBS.

Unfortunately, no data for German STPs was found. According to the “Dringlichkeitsprogramm” of the Federal State Schleswig-Holstein, Germany, from 1989, as threshold of 5 mg/L filterable substances in the effluent has to be met by the 38 hugest STPs in this federal state. On the other hand typical ranges of filterable substances in the effluent have been reported to be 3-30 mg/L (Welker, 2004) or 10-20 mg/L (Baumann, 2003). As data is missing for many member states it could be an option to decrease the concentration of suspended solids to an intermediate level between 7.5 mg/L and 30 mg/L as a realistic conservative assumption.

The separate numerical impact analysis shows no significant effects of the revision of Css from 30 mg/L to 7.5 mg/L for chemicals up to a log Koc of 3, whereas for the two modelled chemicals a reduction of the total emission via the effluent of around 8%, 40% and 70% is predicted for a log Koc of 4, 5 and 6, respectively.

The BPC Environment WG did not agree to the proposed new value of 7.5 mg/L; in the absence of additional information in other countries, the old value of 30 mg/L was therefore kept for biocides.

7. Sewer Removal / (Bio)Degradation Module Inclusion

7.1. Current situation in EUSES

The latest EUSES version i.e. EUSES 2.1.2 (2012) does not include the sewer compartment in the fate evaluation for down the drain chemicals.

7.2. Change proposed (why and what)

Historic laboratory and field studies have shown that sewer degradation is a significant removal process for chemicals disposed down the drain (summaries in Menzies et al, 2017 and Kapo et al 2017) therefore omission of this compartment from EUSES will lead to an incorrect quantification of environmental concentrations for chemicals disposed down the drain. This proposal focuses on the addition of the sewer compartment to the EUSES model.

It is proposed that the sewer model is constructed flexibly such that it can cover several removal processes, ranging from chemical reaction (e.g. reaction of the inorganic oxidant hypochlorite with sulphides in the sewer), to hydrolysis and biodegradation for organic chemicals. Removal by sorption and settling should not be included. Similar to the SimpleTreat model, the sewer model will calculate primary removal (i.e. parent removal) and both models can therefore directly be coupled.

Implementation of this module in its simplest form, could be just a correction factor (% removed in sewer – with the default being zero). At the next level, the sewer removal could be modelled for the chemical (i.e. specific reaction, hydrolysis or biodegradation rate) and residence time based on typical values for region or country. The reaction rate will typically be a first order rate constant.

In-sewer biodegradation rate data can be obtained for any chemical by evaluating the chemical in an OECD 314A Sewer Water Die-Away. This method can be used to quantify primary and ultimate biodegradation rates as well as metabolite formation and decay. Menzies et al (2017) recently applied this method to a suite of nonionic and anionic surfactants and quantified rates of primary and ultimate biodegradation.

Sewer transit time also needs to be thoroughly evaluated in order to add this compartment to EUSES. A robust study by Ort et al., 2014 reported sewer transit times (obtained by survey data for facilities) for 31 wastewater treatment facilities across Europe. The average sewer transit time was 4.6 hr, minimum was 1 hr, and maximum was 12 hr. This data could be leveraged for sewer transit time estimations in the EUSES update.

In addition, sewer residence times from monitoring studies for specific wastewater facilities have been reported for parts of Europe, including the UK (mean 2 h) and Rome (3–5 h) (Johnson and Williams, 2004). Kapo et al. (2017) recently completed a robust assessment of sewer transit times in the US and found that the mean travel time was 3.3 hrs. These data sets further support the data provided in the Ort et al. (2014) study.

7.3. Priority level

For the implementation of new sewer module in EUSES:

1. Number (type of) of chemicals affected- all chemicals that are disposed of down the drain and degrade in a sewer.
2. PECs for all chemicals will be refined with this addition.
3. The need for inclusion of the sewer module is well documented in the literature.
4. An OECD method already exists for assessing chemical biodegradability in the sewer (OECD 314A).
5. Regulatory considerations: no impact on the regulation.
6. New data requirement: data on reaction in sewer needed.

Suggested priority:

Ready and high importance for ECETOC, since the proposed change will bring in the sewer compartment making EUSES more accurate for chemicals disposed down the drain.

ECHA acknowledge that such calculations are done for specific cases for biocides (rapidly reacting substances using the equation of ESD for PT5) but considers that more discussion is needed on the boundaries for such implementation. Indeed we need to ensure that degradation is not overestimated by duplicating assumption on removal processes

7.4. References

Johnson, A.C., Williams, R.J., 2004. A model to estimate influent and effluent concentrations of estradiol, estrone and ethinylestradiol at sewage treatment works. Environ. Sci. Technol. 38, 3649–3658.

Kapo, KE, Paschka M, Vamshi R, Sebasky M, McDonough K. 2017. Estimation of U.S. sewer residence time distributions for national-scale assessment of down-the-drain chemicals. Science of the Total Environment 603-604: 445-452.

Menzies, J., McDonough, K., McAvoy, D. Federle, T. 2017. Biodegradation of Nonionic and Anionic Surfactants in Domestic Wastewater under Simulated Sewer Conditions. Biodegradation. 28(1): 1-14.

Ort, C., van Nuijs, A.L.N., Berset, J., Bijlsma, L., Castiglioni, S., Covaci, A., de Voogt, P., Emke, E., Fatta-Kassinos, D., Griffiths, P., Hernandez, F., Gonzalez-Marino, I., Grabic, R., Kasprzyk-Hordern, B., Mastroianni, N., Meierjohann, A., Nefau, T., Ostman, M., Pico, Y., Racamonde, I., Reid, M., Slobodnik, J., Terzic, S., Thomaidis, N., Thomas, K.V. 2014. Spatial differences and temporal changes in illicit drug use in Europe quantified by wastewater analysis. Addiction 109 (8), 1338–1352.

8. Enhancing the potential for site-specific assessment for the atmospheric compartment

8.1. Current situation in EUSES

Currently EUSES is used mainly for a generic environmental assessment under REACH registration process. However, in some cases it is also used as a tool for site-specific environmental exposure assessment e.g. when assessing own site (e.g. manufacturing site) for registration or in an application for authorisation (AfA).

Some of the improvements proposed for EUSES update, like for example the implementation of simpletreat 4.0, will enhance the potential for EUSES to be used for site-specific assessment (in this case, simulating an industrial biological waste water treatment plant). Moreover, EUSES is already sufficiently flexible to take some site-specific considerations into account (e.g. specific food intake values for a local assessment).

However several refinements are needed to allow an improved site-specific assessment for the atmospheric compartment.

In particular, the calculation used to estimate PEClocal air is based on a standard factor derived from the results of Gaussian plume modelling undertaken during EUSES development (OPS) assuming various standard conditions, including meteorological conditions. As such, plume modelling is not present in EUSES and relevant conditions cannot be changed by the user. Based on the standard factor, the model estimates a concentration in air (at 100 m from the source) and deposition to soil (at 1000 m from the source) using only the emission to air (kg/day). The standard conditions used during the development of EUSES were:

- Stack height: 10 m
- Stack diameter 0.5 m
- Gas velocity: 0.1 m/s
- Gas exit temperature: 20 C (no heat content)

The meteorological conditions were neutral with a wind speed of 3 m/s. The conditions used during model development were conservative (e.g. low height of the emission no heat content in emitting gas, etc.).

8.2. Change proposed (why, what)

The proposed change is to enable site-specific assessments where the conditions are less conservative than those used when EUSES was developed (not top down assessment). Various approaches based on similar Gaussian models are already frequently used by applicants during the authorisation process, but they have to be undertaken outside of EUSES and then output of external models connected to EUSES to estimate exposure of humans via environment.

We therefore propose to implement the same OPS Gaussian model used in EUSES development, and enable the user to change the default values of the parameters listed above to more closely reflect their “site specific” conditions, including also the distance from the point source at which the PEClocal is calculated. In this way a user is able to estimate a less conservative concentration in air and deposition to soil based on their site-specific emission conditions.

8.3. Support for implementation

The model we propose to implement is described and applied in an excel factsheet :

- RIVM OPS model: https://www.infomil.nl/onderwerpen/lucht-water/lucht/zeer-zorgwekkende/immissietoets/beperkte/

8.4. Priority level

Criteria for priority evaluation:

1. Chemicals affected: not substance specific; however it might be used in a limited number of cases (only for site-specific assessment)
2. Expected impact on exposure and/or alternative solutions available: important impact on exposure estimates (can be an order of magnitude different compared to the current EUSES implementation) in case of site-specific assessment. Alternative models do exist (RIVM excel tool, other Gaussian models), but then the outputs need to be connected to EUSES to calculate subsequent exposure (soil concentration, exposure of humans via environment).
3. Maturity of the improvement: the change is well documented (OPS tool, Gaussian models, etc.) and mature for implementation
4. Implementation in IT tools: the model we propose to add in EUSES is already implemented in excel sheet (RIVM).
5. Regulatory considerations: no impact on the regulation. The model is the same as described in R16 guidance. Only its flexibility is enhanced here.
6. New data requirement: no new data needed in term of substance properties. Only site specific emission parameters needs to be specified.

Suggested priority: Technically ready (see below); medium importance

Medium priority since the proposed change only affects site specific assessment (e.g. under AfA process) where work around (use external tool and connect outputs to EUSES) is possible; Ready for implementation as the model is already available and consistent with the existing guidance.

Note that the current OPS model is different than the one implemented in EUSES. Therefore if the current OPS model would be used to overwrite the implementation in EUSES this would affect the exposure in all cases. The impact of such change needs to be further assessed.

9. Local soil deposition of gaseous substances

9.1. Current situation in EUSES

In EUSES the deposition flux to soil consists of the deposition of gas/vapour and deposition of aerosols. A correction is applied for the fraction of the substance bound to aerosols based on the Junge equation (EC, 2004). The deposition of aerosols and of the gaseous fraction includes both wet and dry deposition as depicted in Figure 5.

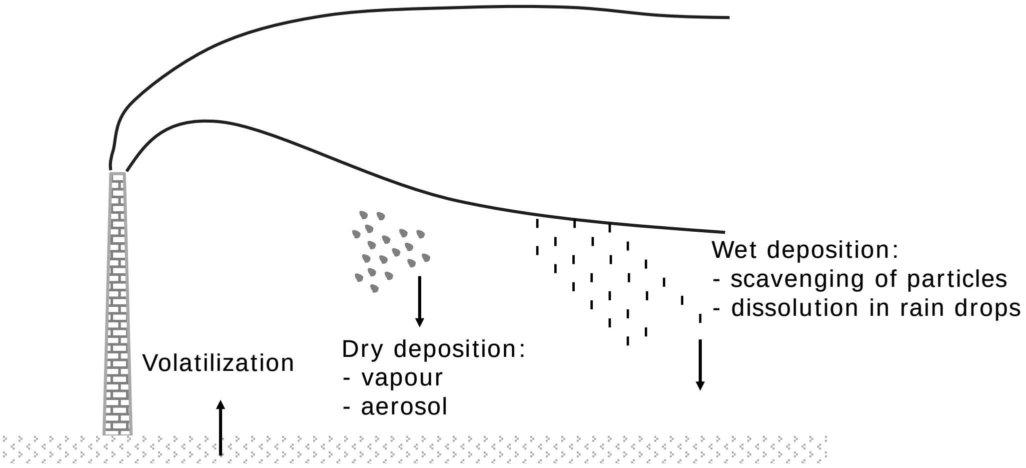


Figure 5: Wet and dry deposition processes of gaseous and aerosol bound compounds in EUSES.

To calculate the deposition to soil EUSES applies standard deposition factors.

These standard deposition factors are determined with the OPS model (Toet and de Leeuw, 1992). Calculations were carried out for both gaseous and aerosol-bound phase. These calculations were carried out for a source strength of 1 kg.s-1, as it has been shown that concentrations and deposition fluxes are proportional to the source strength (Toet and de Leeuw, 1992).

The total deposition rate is calculated from the emission rate according to the following equation:

The total deposition rate is calculated from the emission rate according to the following equation:

$$DEPtotal = \left(Elocal_{air} + Estp_{air} \right) \cdot \left(Fass_{aer} \cdot DEPstd_{aer} + (1 - Fass_{aer}) \cdot DEPstd_{gas} \right)$$

Where:

DEPtotal = total deposition flux (kg.m^{-2}.d^{-1})

Elocal$_{air}$ = emission rate to air (kg.d^{-1})

Estp$_{air}$= indirect emission rate to air from STP (kg.d^{-1})

Fass$_{aer}$ = fraction of the chemical bound to aerosol

DEPstd$_{aer}$ = standard deposition flux of aerosol-bound compounds at a source strength of 1 kg.d^{-1} (kg.m^{-2}.d^{-1})

DEPstd$_{gas}$ = standard deposition flux of gaseous compounds as a function of the Henry coefficient at a source strength of 1 kg.d^{-1} (kg.m^{-2}.d^{-1})

The standard deposition flux for aerosol-bound fraction is 10^{-8} kg.m^{-2}.d^{-1} at a source strength of 1 kg.d^{-1}. The standard deposition flux for gaseous fraction is a function of Henry's Law coefficient as presented in Table 1.

Table 1: Deposition flux of gaseous compounds as a function of Henry's Law coefficient.

deposition flux of gaseous compounds at 1 kg.d^{-1}	DEPstd$_{gas}$	[kg$_c$.m^{-2}.d^{-1}]	
^{10}log HENRY < -2			5.10^{-10}
-2 < ^{10}log HENRY < 2			4.10^{-10}
^{10}log HENRY > 2			3.10^{-10}

Independently from the local air concentration, the volatilization of compounds from soil is calculated in EUSES. This should be seen as a loss process for the local soil compartment. The volatilization from soil has no influence on the local air concentration. The local air concentration is calculated independently using a standard conversion factor at source strength.

It appeared from calculations with the EU TGD spreadsheet version that the local soil concentrations for gaseous substances, emitted to air are unexpectedly high. ECETOC reported this issue and requested to adjust EUSES. This issue was included in the EUSES blacklist.

The issue has been analysed and from the above description of the processes incorporated in EUSES it appears that in principle all relevant exchange processes are included with respect to the soil compartment such as wet and dry deposition, gas absorption (included in the deposition flux of gaseous compounds) and volatilization.

In the calculation of the deposition via aerosols, the fraction of the chemical bound to aerosols is included. For very volatile chemicals this fraction will be very small and leading to a negligible deposition rate compared to the gaseous deposition.

This leads to the conclusion that the problem is caused by the standard deposition factor for gaseous compounds, which has a default value of 3.10^{-10} kg.m^{-2}.d^{-1}. This value is probably too high for very volatile substances with very high Henry's Low coefficients.

The standard deposition for the gaseous fraction is the sum of wet deposition and dry deposition of gases. Wet deposition depends on the gas partitioning between air and rain drops (wash-out ratio). Dry deposition of gases or gas absorption is a diffusive process. The dry deposition velocity is set at a fixed rate of 0.01 cm.s^{-1}. For very volatile chemicals with a Henry's Law constant > 100 the wet deposition is negligible and the deposition rate will be proportional with the dry deposition velocity.

9.2. Change proposed (what)

It is suggested to refine the standard deposition flux for gases by introducing a substance dependent dry deposition velocity. The new standard deposition fluxes could be estimated with the OPS-model or the factors could be refined outside OPS using an appropriate method to calculate the substance dependent dry deposition velocity.

9.3. Why to propose such change

The local soil concentrations for gaseous substances are too high for very volatile chemicals emitted to the local air and therefore this need to be corrected. This will influence the predicted local concentrations in soil as well as the indirect exposure for man via the environment such as the concentrations in meat and dairy products and the plant uptake via roots. Local air and water concentrations will not be affected.

No additional input is required and no additional output will be generated. Only some additional default factors will be added to assess the dry deposition rate for gaseous substances.

9.4. Priority level

Criteria for priority evaluation:

1. Chemicals affected (type, number): The proposed changes would affect substances with high vapour pressures and/or low water solubilities, i.e. substances with high air-water partition coefficients, which is the case for chemicals that are in gaseous form at ambient pressure and temperature. It would affect other extremely volatile chemicals as well.
2. Expected impact on exposure and/or alternative solutions available: The impact may be large. The updated would lead to considerably lower concentrations in soil. Consequently the uptake in plants (roots) and cattle in the man via the environment exposure

assessment although these exposure routes are usually not very relevant for very volatile organic compounds. Alternatively the problem of local PECs in soil can be solved by applying multimedia mass balance calculation of local PECs, as done for the larger spatial scales. This proposal is further elaborated in section 15. Implementation of that change in EUSES is to be considered a relatively large effort (ECHA, 2014).

3. Maturity of the improvement (e.g. scientifically documented/ further research needed): Proposed method is a refinement of the existing factors used. An additional factor to account for the deposition of gaseous compounds in will be introduced in EUSES. The calculation procedure will remain unchanged. The deposition factors have to be determined with the latest version of the OPS Model (Sauter et al., 2018) or alternatively by applying another appropriate method to calculate the substance dependent dry deposition velocity.
4. Implementation in IT tools: Methods to derive the dry deposition velocity are provided in Simplebox and the OPS model
5. Regulatory considerations: Not relevant
6. New data requirement: No new data is required.

Suggested priority: not ready; important

The proposed change is considered important because the impact on the calculated local soil concentrations would be large as the proposed change would lead to considerably lower concentrations in soil. The implementation in EUSES would require minimal effort. Some preparatory work has to be done such as generating new defaults with the OPS, though.

For very volatile substance the local soil concentrations are overestimated. For these kind of substances the default dry deposition velocity in EUSES is too high and these need to be corrected. The impact may be large as the proposed change would lead to considerably lower concentrations in soil. Existing defaults should be updated and additional classes with new defaults should be added for the standard deposition rate of gaseous compounds.

9.5. References

EC (2004) European Union System for the Evaluation of Substances 2.0 (EUSES 2.0). Prepared for the European Chemicals Bureau by the National Institute of Public Health and the Environment (RIVM), Bilthoven, The Netherlands (RIVM Report no. 601900005).

Toet C, De Leeuw FAAM. 1992. Risk assessment system for new chemical substances: Implementation of atmospheric transport of organic compounds. RIVM Report 679102008. National Institute for Public Health and the Environment (RIVM), Bilthoven, The Netherlands.

Sauter F, van Zanten F, van der Swaluw E, Aben J, de Leeuw F, van Jaarsveld H (2018). The OPS-model, Description of OPS 4.5.2. National Institute for Public Health and the Environment (RIVM).

ECHA (2014). Identification and preliminary analysis of update needs for EUSES. CONTRACT NO. ECHA/2014/253. Dik van de Meent, Joris Quik, Theo Traas. 12/22/2014. National Institute of Public Health and the Environment (RIVM) Bilthoven, The Netherlands

10. Episodic Rain / Extremely soluble chemicals

10.1. Current situation in EUSES

Most multimedia fate models, including the exposure modelling in EUSES, assume atmospheric deposition to be continuous (i.e. at one constant rate all the time). This is unrealistic, as wet deposition (wash-out, rain-out) occurs only during relatively short rain episodes and not as a constant ‘drizzle’.

10.2. Change proposed (why and what)

Because of the assumed constant atmospheric deposition the current EUSES model description does not predict atmospheric fate of extremely soluble chemicals correctly.

A model formulation has been worked out and published (Jolliet and Hauschild, 2006) that represents episodic rainfall. Wet deposition will be higher during rain events, while during the intermediate periods there is only dry deposition and concentrations in air will build up (Figure 6). The hypothesis of continuous rain for instance for hydrophilic substances leads to a considerable underestimation of the residence time and travel distance for relatively volatile chemicals (Jolliet and Hauschild, 2006). The developed approximation is designed to be implemented in multimedia models and provides improved precision between steady-state and complex dynamic models. The proposed model calculations can be easily implemented in existing multimedia mass balance models. It is proposed to replace the current EUSES model description of wet deposition by Jolliet and Hauschild's episodic rain model as done already in SimpleBox4.0 (Hollander et al., 2016).

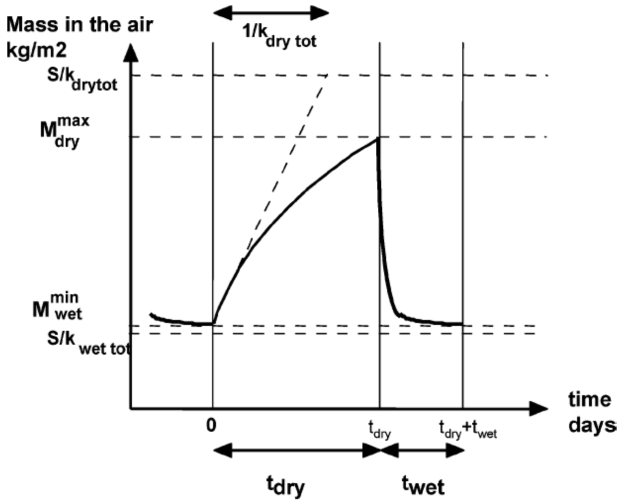


FIGURE 2. Mass of substance present in the air compartment as a function of dry and wet deposition under a regime of intermittent precipitation.

Figure 6 from (Jolliet and Hauschild, 2006)

The proposed change will affect predicted concentrations in air, water and soil at the larger spatial scales, the local concentrations would not be affected. Especially chemicals with a relatively high water solubility and/or low vapor pressure, i.e. substances with high air-water partition coefficients that are released in air, the proposed model would predict considerably lower concentrations in air, and higher concentrations in soil and water. A sizeable number of chemicals such as organic (and inorganic) acids with a pKa value below 6 such as carboxylic and sulphonic acids and their permanently charged anionic salt species would be affected.

10.3. Support for implementation

SimpleBox 4.0 is available via

http://www.rivm.nl/en/Topics/S/Soil_and_water/SimpleBox_4_0_tool

10.4. Priority level

Criteria for priority evaluation:

1. Chemicals affected: sizeable number of chemicals, mainly organic and inorganic acids with a pKa < 6 and their salts.
2. Expected impact on exposure and/or alternative solutions available: Residence time and long range transport in air will be considerably affected depending on substance properties as well as calculated deposition rates to soil and surface water.
3. Maturity of the improvement (e.g. scientifically documented/ further research needed): Method is scientifically documented and verified for a limited number of chemicals.
4. Implementation in IT tools: method is implemented in SimpleBox 4.0
5. Regulatory considerations: no
6. New data requirement? No additional input is required and no new output generated.

Suggested priority: Ready/Low importance

Method is ready to be implemented and will have large impact on the predicted concentrations in air, water and soil on the regional scale for chemicals released to air. The local predicted concentrations would not be affected.

The proposed method is documented and verified for a limited number of chemicals (Jolliet and Hauschild, 2005) and it is implemented in SimpleBox 4.0 (Schoorl et al., 2014). In principle no additional input is required and the output is not changed. It will affect a sizeable number of chemicals such as organic acids and permanently charged anionic salt species. The impact on the exposure calculation is expected to be relatively high, depending on the substance properties but especially for chemicals with a relatively high water solubility and/or low vapour pressure.

10.5. References

Jolliet O and Hauschild M (2005). Modelling the Influence of Intermittent Rain Events on Long-Term Fate and Transport of Organic Air Pollutants. Environ. Sci. Technol. 39, 4513-4522

Schoorl M, Hollander A, Van de Meent D (2014). SimpleBox 4.0: A multimedia mass balance model for evaluating the fate of chemical substances. RIVM Report 2015-0161.

11. Assessment of photolytic degradation

11.1. Current situation in EUSES

Current EUSES offers users who prepare REACH registrations the possibility to account for photolytic degradation of chemical substances by entering an environmental half-life for photolysis. Photolysis half-life under real environmental conditions is often hard to find in (literature) reports on photolysis studies. Often, no more than half-lives of pure chemicals in water, measured with artificial light sources, under laboratory conditions are readily available to risk assessors (OECD, 2008).

The current EUSES model requires registrants to enter field-specific half-lives of chemicals due to direct or indirect photolytic degradation in water, without assistance offered from the model. This limits the applicability of EUSES for including the influence of photodegradation on environmental half-lives of persistent, but potentially photolabile, chemicals such as for instance some polycyclic aromatic hydrocarbons, brominated flame retardants, pesticides and antibiotics.

11.2. Change proposed (why and what)

Castro Jiménez and Van de Meent (2011) have reviewed the available literature on photolytic degradation of chemical substances under environmental conditions and have proposed a calculation tool to derive the environmentally relevant half-lives in water that EUSES accepts as input.

By implementing the formulations suggested by Castro Jiménez in EUSES risk assessors will be able to predict exposure concentrations, using only the information available from technical studies that report results of the standard photolysis test (OECD, 2008).

Implementation of this change would offer risk assessors the option to evaluate for instance the influence of photodegradation on persistent chemicals that are only photolytically degradable. This is an element in the ‘P’ assessment of chemicals where environmental fate can be studied using fate modelling, supporting e.g. further P(BT) assessment for REACH.

The proposed change will only influence the exposure concentrations in water and indirectly in sediment at the larger (regional) spatial scales in principal for all chemicals that may undergo photolytic breakdown in the environment. Photodegradation is not included in the local exposure calculations. It will not affect the elimination of the substance that may take place in in the STP, soil or sediment because abiotic degradation is not estimated for these compartments.

EUSES needs as input, the half-lives or rate constants measured under laboratory conditions according to (OECD, 2008),. No additional output will be generated (unless the user is interested in the generated ‘field relevant half-life for phototransformation’).

Castro Jiménez and Van de Meent (2011) tested the proposed formulations by implementing them in SimpleBox vs. 3, available from the authors. This implementation can be integrally copied into the EUSES fate model calculations.

11.3. Support for implementation

The proposed formulations are implemented in a test version of SimpleBox vs. 3 (Castro and Van de Meent, 2011) and available from the authors.

11.4. Priority level

Criteria for priority evaluation:

1. Chemicals affected: Mainly a small number of photolytically degradable chemicals that are persistent to biodegradation
2. Expected impact on exposure and/or alternative solutions available: Relatively low. It is expected that the outcome will usually be that photolysis will not be relevant under field conditions for persistent chemicals. However, the transfer from lab to field-relevant rates will be supportive for the P assessment.
3. Maturity of the improvement (e.g. scientifically documented/ further research needed): Documented

4. Implementation in IT tools: Not implemented in a publicly available model. Algorithms are implemented in a test version of Simplebox 3.0.
5. Regulatory considerations: The tool will be supportive in the assessment of persistency of potential PBT or vPvB substances.
6. New data requirement? no

Suggested priority: Technically ready/ Low importance

The proposed method is ready to be implemented.

Importance is judged to be low because photolysis data are only for a small number of chemicals and it affects the concentrations only at the higher spatial scales. It will only affect the higher spatial scales in EUSES for a small number of chemicals. Impact on exposure is expected to be relatively low and often not very relevant under field conditions (Castro Jiménez J and Van de Meent D, 2011). It may be relevant for chemicals that are persistent to biodegradation but readily degradable by photolysis though.

11.5. Open question

Relevance of photolysis under field conditions is questioned. Are there any new insights with respect to the relevance under field conditions?

11.6. References

Castro Jiménez J and Van de Meent D (2011). Accounting for photodegradation in P-assessment of chemicals. Radboud University Nijmegen. Reports Environmental Science no 381, 2011. 20

OECD (2008). Guidelines for the testing of chemicals. Phototransformation of Chemicals in Water – Direct Photolysis (TG 216, adopted 3 oct. 2008), OECD Paris, France.

Den Hollander HA, van Eijkeren JCH and Van de Meent D (2004). SimpleBox 3.0: multimedia mass balance model for evaluating the fate of chemical in the environment. RIVM report 601200003/2004

ECETOC (2013) Assessing Environmental Persistency, 6-7 November 2012, Paris. Workshop Report No. 24. Brussels, December 2013.

12. Providing a new concentration in soil for indirect release: PEC soil initial

12.1. Current situation in EUSES

The PEC in soil (e.g. following sewage sludge application) is calculated as an averaged value over 30 days after the last sewage sludge application. Also the concentration averaged over 180 days is available and used as input for exposure of predators (secondary poisoning) and man via the environment. Note that for the application of sewage sludge it is assumed as a realistic worst-case that sewage sludge application takes place for 10 consecutive years.

12.2. Change proposed (why and what)

When performing risk assessment for the terrestrial compartment, care should be taken that the PEC and PNEC soil are based on comparable exposure patterns. This means that degradation of the substance in the soil should be consistently taken into account in both the exposure (PEC) and effect (PNEC) parameters.

When degradation is not taken into account to derive the PNEC (as the results of currently available standardised terrestrial ecotoxicity tests are generally expressed on the basis of initial, nominal concentrations in test with single applications) it has been agreed for the assessment in biocides (and this is reflected in the current guidance[16]) that the PNECsoil should be compared with the *initial PECsoil*, which is the PECsoil directly after the last sludge application (before degradation takes place).

Therefore we suggest that EUSES should provide both the *initial PEC in soil* (immediately after the last application) in addition to the *30 days (and 180 days) average PEC* (average PEC over a period of 30/180 days after the last application). The 30 days averaged PEC is to be used when the PNECsoil is representative for time averaged exposure concentrations too. This may for example be the case if the PNECsoil is derived by equilibrium partitioning from a PNECaquatic for chronic exposure, where the PNECaquatic is based on study results that are expressed as time averaged concentrations.

The same principle is applied for biocides also when calculating the exposure from application of manure (containing biocides following to stable applications) to agricultural land.

The above procedure was so far not yet discussed for REACH and is currently only applicable to biocides. With regard to the implementation in EUSES, there could be a flexible way implementation calculating two different PEC values, to allow the assessment of different PEC values for biocides.

12.3. Support for implementation

The equations to build the model calculations in EUSES accordingly are provided in the following document:

- Guidance on the Biocidal Products Regulation - Volume IV Environment - Assessment and Evaluation (Parts B + C), Version 2.0 (October 2017) – section 2.3.7.5.1 (page 90)

12.4. Priority level

Criteria for priority evaluation:

1. Number (type of) of chemicals affected: option that can be used for all chemicals if wished
2. Expected impact on exposure: A possibility to calculate initial PEC/average PEC values needs to be implemented.
3. Maturity of the improvement: the changes are documented in current biocides guidance (Guidance on the Biocidal Products Regulation - Volume IV Environment - Assessment and Evaluation (Parts B + C).
4. Implementation in IT tools: so far not implemented.

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[16] https://echa.europa.eu/documents/10162/23036412/bpr_guidance_ra_vol_iv_part_b-c_en.pdf/e2622aea-0b93-493f-85a3-f9cb42be16ae

5. Regulatory considerations: no impact on the regulation for biocides since the proposed changes are already agreed by the relevant regulatory body (i.e. the BPC Environment WG). For REACh, this approach does not exist so far.
6. New data requirement: no new data needed.

<u>Suggested priority:</u> ready/ high importance

Such PEC is now required for biocides

13. Depth-dependent concentration in soil

13.1. Current situation in EUSES

Multimedia mass balance models typically assume compartments to be well-mixed, have a fixed volume, depth or height, and that all processes obey first-order kinetics. This is also the case for soils. Calculated concentrations are therefore the same throughout the whole compartment. In reality soils are usually poorly mixed across depth and concentrations of pollutants usually decrease exponentially with depth, in accord with theoretical understanding. This means that at the soil-air interface, concentrations are found to be higher than the depth-averaged value. At the bottom of the (imaginary) top soil layer, concentrations are usually well below average.

Assuming soils to be well-mixed and having a fixed depth leads to mis-estimation of inter-media transport mechanisms such as absorption, volatilization, run-off and leaching (see Figure 7). Mis-estimation of process rates from soils without accounting for the depth-dependent soil concentration may be large, particularly for chemicals with low or large penetration depths (Hollander et al., 2007). This has been recognized early in the development of multimedia mass balance calculation (Cowan et al., 1995; Brandes et al., 1996; Thibodeaux, 1996). The depth-dependent soil concentration has been implemented as an optional calculation method for estimating the soil side partial mass transfer coefficient at the soil air interface much later in the EUSES 2.0 version on the regional scale (EC, 2004) according to Brandes et al. (1996) which does not yet include the inhomogeneity correction worked out by Hollander et al (2004).

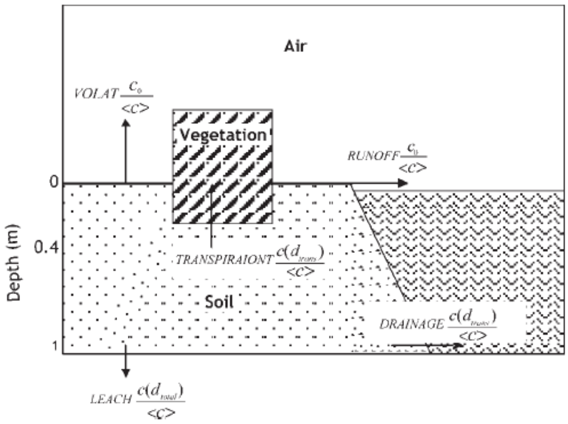


Figure 7: Schematic representation of the processes occurring from the soil compartment in the new Simplebox model (version 4.0) from Hollander et al. (2004).

13.2. Change proposed (why and what)

Hollander et al. (2004) have worked out a correction method, using an inhomogeneity correction factor based on known or theoretically derived penetration depths of substances. Hollander's corrections have been implemented in SimpleBox 4.0 (Schoorl et al., 2014), and are proposed here for implementation in EUSES for both the local and regional scale. The standard depths as defined in EUSES will not change and no new input is required.

Transport processes take place at a certain depth (z) rather than over the average soil depth. The concentration at a certain depth, c(z) can be calculated from the average concentration <c> over the standard depth in EUSES according to the following equation:

$$c(z) = \langle c \rangle \frac{d_t/d_p}{1 - e^{(-d_t/d_p)}} e^{(-z/d_p)}$$

Where

d_t is the total depth, or the fixed soil depth in EUSES

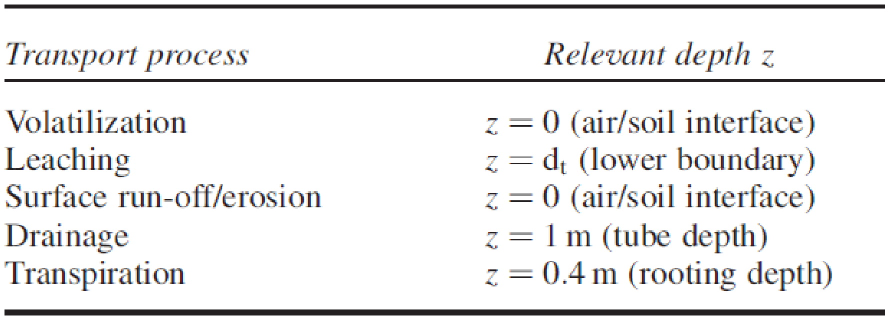
d_p is the chemical dependent characteristic soil (penetration) depth z is the depth were transport process take place

The transport coefficients are corrected by applying the correction factor is c(z) / <c>:

$$\frac{d_t/d_p}{1-e^{(-d_t/d_p)}}e^{(-z/d_p)}$$

To implement the correction method relevant depths have to be defined for each fate process, such as volatilization, leaching and uptake by root crops at both the local and regional scale, see Table 3.

Table 3 : relevant depths for the various transport processes as defined in Simplebox 4.0 (Hollander et al, 2004)



Transport process	*Relevant depth z*
Volatilization	$z = 0$ (air/soil interface)
Leaching	$z = d_t$ (lower boundary)
Surface run-off/erosion	$z = 0$ (air/soil interface)
Drainage	$z = 1$ m (tube depth)
Transpiration	$z = 0.4$ m (rooting depth)

As an example the correction method is elaborated for the volatilization from soil at the local scale. The overall removal-rate constant for the local soil is given by the sum of all relevant-removal rate constants:

$$\boldsymbol{k_i = k_{volat\,i} + k_{leach\,i} + kdeg_{soil}}$$

In which

K_{volat} is the volatilization rate constant [d^{-1}]

K_{leach} is the leaching rate constant [d^{-1}]

K_{deg} is the degradation rate constant [d^{-1}]

The rate constant for volatilization is defined as

$$k_{volat} = \frac{kasl_{air} \cdot kasl_{soil}}{kasl_{air} + kasl_{soil} \cdot K_{soil-water}/K_{air-water}} \cdot \frac{CORR}{DEPTH}$$

Where:

kaslsoil	partial mass-transfer coefficient soil side of air-soil interface	[$m.d^{-1}$]
kaslair	partial mass-transfer coefficient air side of air-soil interface	[$m.d^{-1}$]
Kair-water	air-water partition coefficient	[$m^3.m^{-3}$]
Ksoil-water	soil-water partition coefficient	[$m^3.m^{-3}$]
DEPTHi	the mixing depth of the soil compartment	[m]
CORR	Correction factor for the transport rate constant	[-]

$$CORR_{volat} = \frac{DEPTH/d_p}{1 - e^{(-DEPTH/d_p)}}$$

The depth z disappears from the equation for the correction factor, because volatilization takes place at the soil surface and z = 0.

The proposed change will affect in principal all types of chemicals. The largest effects should be anticipated for substances that penetrate to small depths only, so that average concentrations in soil are much smaller than concentrations at the soil-air interface. Small penetration depths are expected (and observed) for substances that strongly adsorb to the solid phase of soil and/or rapidly degrade. The reverse will hold for very mobile chemicals with large soil penetration depths.

13.3. Support for implementation

SimpleBox 4.0 is available via
http://www.rivm.nl/en/Topics/S/Soil_and_water/SimpleBox

13.4. Priority level

Criteria for priority evaluation:

1. Chemicals affected: The proposed change affects a sizeable number of chemicals especially those strongly absorbing and/or rapidly degrade and those that are very mobile in soil
2. Expected impact on exposure and/or alternative solutions available: impact on exposure on both the regional and local scale can be large depending on a combination of substance properties
3. Maturity of the improvement (e.g. scientifically documented/ further research needed): Method is scientifically documented no further research needs
4. Implementation in IT tools: method implemented in SimpleBox 4.0
5. Regulatory considerations: no
6. New data requirement? Diffusion coefficients needed to estimate the characteristic soil depth can be calculated from the molecular weight. Alternatively substance specific diffusion coefficients for air and water can be used as input. These are available from handbooks.

Suggested priority: Ready/High importance

Method is ready to be implemented and is important because mis-estimation of process rates from soils without depth-dependent soil concentration may be large at both the regional and local scale.

The proposed method is documented, verified (Hollander, 2004) and implemented in SimpleBox 4.0. In principle no additional input is required and the output is not changed. It will affect all types of chemicals. The impact on the exposure calculation for both the local and regional scale is expected to by high, mostly for substances that strongly adsorb to the solid phase of soil and/or rapidly degrade.

13.5. References

Brandes LJ, Den Hollander AH, Van de Meent D. 1996. SimpleBox 2.0: a nested multimedia fate model for evaluating the environmental fate of chemicals. Bilthoven, RIVM report 719101 029

Cowan C, Mackay D, Feijtel T, Van de Meent D, Di Guardo A, Davies J, Mackay N. 1995. The multimedia model: a vital tool for predicting the fate of chemicals. SETAC Press, Pensacola FL, USA.

Hollander A, Hessels L, De Voogt P, Van de Meent D. 2004. Implementation of depth-dependent soil concentrations in multimedia mass balance models. SAR and QSAR in Environmental Research 15, 457-468.

Hollander A, Baijens I, Ragas A, Huijbregts M, Van de Meent D. 2007. Validation of predicted exponential concentration profiles of chemicals in soils. Environmental Pollution 147, 757-763.

EC (2004) European Union System for the Evaluation of Substances 2.0 (EUSES 2.0). Prepared for the European Chemicals Bureau by the National Institute of Public Health and the Environment (RIVM), Bilthoven, The Netherlands (RIVM Report no. 601900005).

Schoorl M, Hollander A, Van de Meent D (2014). SimpleBox 4.0: A multimedia mass balance model for evaluating the fate of chemical substances. RIVM Report 2015-0161.

Thibodeaux LJ. 1996. Environmental chemodynamics: movement of chemicals in air, water and soil. New York, Wiley, 1996.

14. Different Kp(susp) and Kp(sed) for seawater and freshwater

14.1. Current situation in EUSES

Currently, EUSES does not differentiate the following partitioning coefficients between freshwater and seawater (both at local and regional scale):

- *Solids-water partition coefficient sediment (Kp.sed, L/kg)*
- *Solids-water partition coefficient suspended matter solids (Kp.sus, L/kg)*

Furthermore, for the local situation, there is no differentiation made between the fresh and marine water environment with respect to the compartment characteristics (volume fraction water, solids and weight fraction organic carbon). Note that for the local situation, only suspended matter characteristics are relevant.

For the larger scales (regional and continental), there is no differentiation between fresh and marine environment in EUSES. Only the concentration of suspended solids differs between freshwater (15 mg/L) and seawater (5 mg/L).

14.2. Change proposed (what)

Option 1: Include separate Kp(susp) and Kp(sed) for marine environment (short term)

It is proposed to adjust EUSES to allow entry of separate Kp values for marine and freshwater environments (for all scales). By default, marine Kp values are set equal to freshwater Kp values (as currently assumed in EUSES).

It should be able to overwrite the default partitions coefficients values with partition coefficients based on measured values. This option would only impact chemicals that have information on Kp for marine environment.

Option 2: Improve the environmental characteristics of the marine water and sediment compartments in order to improve default calculation of the Kp(susp) and Kp(sed) for marine environment (long term)

A local fresh and marine environment should be distinguished with different suspended matter characteristics. This may allow to calculate separate (default) partition coefficients (suspended matter only) for the marine environment. The additional compartment characteristics (mainly organic carbon content for suspended matter and sediment) for the larger scales should be displayed as separate defaults in EUSES.

A differentiation will also be needed between ionizable and non-ionizable chemicals. For ionising substances, it needs to be clarified:

- If the new QSARs now proposed for ionising substances apply to both fresh and marine water, with the only difference of the pH marine and fresh that determines different Koc for marine and fresh
- Or if new QSARs for Koc determination are required for marine water.

This option potentially affects all chemicals but more likely ionizable chemicals.

14.3. Why to propose such change

The possibility to have 2 different partitioning coefficients Kp (sediment, suspended solid) for marine and freshwater would allow to differentiate for substances where different partitioning behaviour is expected between sea water and freshwater (mostly for ionising substances or (metal)salts) due to different ionic strength or pH.

This change would affect water and sediment concentrations (PECs) in the marine part of the local and regional scale, and risk characterisation dependent on it.

In principle, no additional model input would be needed if, by default as in the current EUSES tool, the marine and freshwater partitioning coefficients are calculated in the same way. However, measured Kp's would need to be specified if the user would want to overwrite the "default" Kp's.

14.4. Support for implementation

For option 2, ionic strength impacts the activity coefficients and thus the relation between activity and concentration in MAMI (Franco and Trapp 2010). Only the ionic content of seawater and sediments was found to have a moderate effect on model outputs.

14.5. Priority level

1. Number (type of) of chemicals affected: low number (only those chemicals that have information on Kp in marine water)
2. Maturity: documented: yes for option 1, partly for option 2
3. Implemented into IT tool : not relevant
4. Regulatory considerations : no for option 1, yes for option 2
5. Expected impact on exposure: moderate impact on marine water and marine sediment PEC at regional and local scale.
6. New data requirement: Yes: marine water solid partition coefficient, unless default freshwater solid partition coefficients are used instead.

Suggested priority:

- Option 1: Ready / high importance (low effort)
- Option 2: Not ready/ low importance

14.6. References

Franco, A., Trapp, S. (2010). Multimedia activity model for ionizable compounds - Validation study with 2,4-D, aniline and trimethoprim. Environ. Toxicol. Chem., 29(4), 789–799.

15. Using PEC regional sediment in PEC local sediment calculation

15.1. Current situation in EUSES

The PEC regional sediment is currently not used in the PEC local sediment calculation. Instead, the PEC regional, sediment is calculated based on PEC regional, water and partitioning. This way of calculating local concentrations in sediment is in agreement with the spirit of exposure estimation in the TGD. It correctly reflects and implements the influence of regional releases and exposures on local concentrations in sediment and correctly accounts regional influence on local PEC/PNEC ratios in sediment.

Note that PEClocal,sed and PECregional,sed are calculated differently:

- PEClocal,sed based on suspended matter characteristics and
- PECreg,sed based on sediment characteristics

From that perspective the way the regional background is implemented in EUSES is logic and straight forward.

15.2. Change proposed (what)

Current formula: $PEClocal_{sed} = \frac{K_{susp-water}}{RHO_{susp}} \cdot \left(Clocal_{(sea)water} + PECregional_{water}\right) \cdot 1000$

This formula can still remain the default formula.

New formula: $PEClocal_{sed} = \frac{K_{susp-water}}{RHO_{susp}} \cdot Clocal_{(sea)water} \cdot 1000 + PECregional_{sed}$

PEClocal,sed = Clocal,sed + PECregional,sed

This formula would be used in case PECregional,sediment is based on measured data and explicitly inputted.

Changes would affect PEC values at the local scale for sediment, and all corresponding related measures where sediment concentrations are used at the local scale.

No additional input and output is needed, the proposed change only affects calculation of water and sediment concentrations at the local scale (local PECs).

In principle, all substances are potentially affected due to this change but impact is expected to be low because the PECregional is usually negligible compared to Clocal. For metals, the new formulae is already used in REACH registration dossiers, consequently, impact is minimal.

15.3. Why to propose such change

In case PEC regional for sediment is based on measured data (following R.16.4.1.3) and assessed to be more reliable than a modelled PEC regional, this measured PECregional for sediment cannot be used for PEC local sediment (since PEC regional sediment is calculated based on PEC regional aquatic).

15.4. Support for implementation

Implementation follows a simple addition of local and regional scale concentrations, either via addition of local and regional PECs for sediment, or via equilibrium partitioning of the sum of local water and regional water concentrations.

15.5. Priority level

7. Number (type of) of chemicals affected: A large number of chemicals is potentially affected but impact is expected to be low because the PECregional is usually negligible compared to Clocal.
8. Maturity: Scientifically documented: yes
9. Implemented into IT tool : not relevant due to simplicity of equations
10. Regulatory considerations :

11. Expected impact on exposure: Relatively low in the majority of cases due to the expected dominance of local concentrations over regional sediment concentrations.
12. New data requirement: no

Suggested priority: Ready/High importance

15.6. References

EC (2004) European Union System for the Evaluation of Substances 2.0 (EUSES 2.0). Prepared for the European Chemicals Bureau by the National Institute of Public Health and the Environment (RIVM), Bilthoven, The Netherlands (RIVM Report no. 601900005).

EU TGD spreadsheet (2008). Available from Radboud University, Nijmegen NL via http://www.ru.nl/environmentalscience/research/themes-0/risk-assessment/eutgdsheet/

16. Nested local scale model

16.1. Current situation in EUSES

The local scale in the current version of EUSES is modelled as more or less “separate” or “independent” one-compartment models, i.e. the air compartment, freshwater compartment and the soil compartment. The reason is that at the local scale processes are important that are not covered by multimedia models and sometimes can be simplified because of their nature. Air concentrations and deposition fluxes of gaseous and aerosol-bound chemicals are estimated based on a plume model (OPS). A simple linear relationship between source strength and concentration is assumed. The applied constants are calculated with the OPS model using standard setting. Water concentrations are calculated by simple dilution and sediment concentrations are calculated based on the steady-state partitioning outcome of the freshwater compartment. The advantage of the current EUSES local model is that no assumptions are to be made on the volume/mass of the receiving local environment.

16.2. Change proposed (what)

This topic considers a multimedia (i.e. multi-compartment) model (instead of a set of one-compartment models) at local scale whereby:

- The mass balances are closed and made at multimedia level
- Higher tier modelling of local fate processes is possible in PT8 ESD (e.g. consideration of degradation at the local scale). Should also be made possible under standard local STP scenario (under REACH and BPR)
- Where sink processes are included for organics (like degradation), equally sink processes are to be included for inorganics in the sediment and soil compartments (like irreversible binding to minerals = ageing or sediment burial)
- Erroneous high concentration of very volatile substances in soil through atmospheric deposition. The calculated atmospheric deposition flux for gaseous substances is too high.

Given that the proposed change induces significant changes in the conceptual model, two options were developed. The second option refers to a full nested local scale multimedia model and could be seen as a long term objective. The first option identifies a number of useful and relevant items from the full nested local scale model and applies it to the current EUSES local scale model.

<u>Option 1</u>: Improve local scale model by taking improved items from a fully nested local scale multimedia model (in option 2)

Item 1A: Close the mass balance by extending the aquatic one-compartment model at local scale model to a two compartment model (flowing water body: freshwater – sediment)

This item includes the sediment compartment as part of a two-compartment model at the local scale EUSES model, similar to the PT8 ESD static water body scenario, see equation in ESD PT8. A potential consequence is that a default local sediment depth and volume is to be selected. This way, emitted mass is distributed over water and sediment compartment, rather than distribution to water compartment only.

This item is linked to the topic on release scenarios. This item impacts all substances, but more impact expected for highly adsorbing substances.

Item 1B: Consideration of additional fate processes at the local scale

The table below compares the fate processes for the local scale model and the PT8 ESD for the freshwater compartment. In the ESD for PT8, two situations can be distinguished for surface water and sediment: (1) release into a static water body e.g. a lake or pond. This situation corresponds to the scenario for a jetty in a lake. (the regional scale model is added as well for comparison) (2) Release into a flowing water body. This situation corresponds to the scenario for a sheet piling as well as for a wharf on the sea.

	Flowing water body			'Static' water body	
	EUSES	PT 8 ESD		PT 8 ESD	
Fate process	Local scale	Tier 1	Tier 2	Tier 1	Tier 2
Adsorption/desorption suspended matter	**X**		**X**		**X**
Sedimentation and resuspension					To be considered as higher tier
Degradation in water (removal from water column)	To be considered as higher tier?	**X**	**X**	**X**	**X**
Adsorption/desorption sediment	**X**		To be considered as higher tier		**X**
Degradation in sediment					
Sediment burial	To be considered as higher tier?		To be considered as higher tier?		To be considered as higher tier
Irreversible binding to minerals = ageing	To be considered as higher tier?		To be considered as higher tier?		To be considered as higher tier

Following changes are to be considered:

- Include sedimentation and resuspension in Tier 2 of PT8 ESD for static water body: this is a relevant fate process for static water bodies (and partly for flowing water bodies)
- Include higher tier degradation in water in local scale EUSES model, similar to PT8 ESD flowing water body scenario
- Include adsorption/desorption to sediment as part of a two-compartment model at the local scale EUSES model, similar to the PT8 ESD static water body scenario, see equation in ESD PT8
- Include sediment burial and/or irreversible binding to minerals (binding) in PT8 ESD and local EUSES model such that sink processes are included for both organics and inorganics (and not only for organics).

Item 1C: improved air deposition for very volatile substances

The standard atmospheric depositions flux of gaseous compounds depends on the Henry's Law coefficient distinguishing three classes. The standard deposition flux for gaseous compounds of 3.10^{-10} $kg.m^{-2}.d^{-1}$ is to high for very volatile substances with very high Henry's Low coefficients. The standard deposition should be refined flux by incorporating additional classes for very volatile chemicals with a log Henry coefficients up to a value of 6.

Item 1D: nesting local scale model

To be further developed

Option 2: Complete nested local scale multimedia model

This options considers a fully nested multimedia local scale model. An implementation is available and ready-to-use in the spreadsheet version 3.0 of Simplebox (but currently not implemented in EUSES assessments). However, given the conceptual differences with the current local scale model in EUSES, there is a need for further understanding on the improvements as well as the impact on current risk assessments.

	Current EUSES local scale model	*Nested local scale multimedia model*
Mass balance	Closing mass balance	Correctly implemented mass balance in the overall environmental system
Nesting at local scale	No nesting and limited transfer processes between environmental compartments	Different spatial scales are interconnected meaning that there is intercompartmental transport through advective processes between the various spatial scales
Environmental compartment characteristics at the local scale	Limited need to define the volumes and mass of the receiving environmental compartments (only soil is defined)	Need to define the volumes and mass of the receiving environmental compartments

16.3. Why to propose such change

The current local scale model in EUSES overpredicts local freshwater PECs especially for highly adsorbing substances because the sediment compartment is not nested in the local model. Also, erroneous high concentration of very volatile substances in soil through atmospheric deposition is calculated in EUSES. These problems could be solved by a local multi-compartmental boxmodel. The issue on the atmospheric deposition to soil could be solved by adjusting or refining the standard dry deposition velocity for gaseous chemicals. For a more detailed description of this issue see separate topic.

16.4. Support for implementation

- ESD PT8 contains equations in Tier 2 for improved local scale modelling that are applicable to other ESD and REACH scenarios.
- The spreadsheet version 3.0 of Simplebox contains a fully implemented version of a nested local scale model.
- In the framework of an EU research project 4FUN, a state-of-the-art exposure tool MERLIN-Expo (**M**odelling **E**xposure to chemicals for **R**isk assessment: a comprehensive **L**ibrary of multimedia and PBPK models for **I**ntegration, Prediction, u**N**certainty and Sensitivity analysis) was developed. MERLIN-Expo is, compared to EUSES, a more complex model that is typically used in higher tier assessments. MERLIN-Expo tool and its model documentation is freely available at https://merlin-expo.eu/. A scoping exercise would be need to identify further scientific improvements for EUSES.

16.5. Priority level

1. Number (type of) of chemicals affected: for option 2: all chemicals; for option 1: depends on the item
2. Maturity: from the scientific perspective: very well documented but relatively new from the regulatory perspective
3. Implemented into IT tool: Yes, SimpleBox, MERLIN-Expo, ESD PT8, etc…
4. Regulatory considerations: Yes, needed. A nested local scale multi compartmental box model would generate very different results depending on the extent to which the new local scale model can be parameterised to match the results of the current model. From a chemicals regulation point of view this would be a highly undesirable situation.
5. Expected impact on exposure: high for option 2, for option 1: depends on the item
6. New data requirement: currently none identified.

Suggested priority:

- Option 1: Technically ready but impact may be non desired, high importance
- Option 2: Technically ready but impact may be non desired, low importance

17. Man indirectly exposed via the environment

17.1. Current situation in EUSES

Indirect exposure of humans via the environment may occur by consumption of food and drinking water, inhalation of air and ingestion of soil. In EUSES humans are indirectly exposed to the environment via the intake of food (meat, fish, crops and dairy products) the inhalation of air and via drinking water. The different routes of exposure that are taken into account in EUSES are shown in Figure 8.

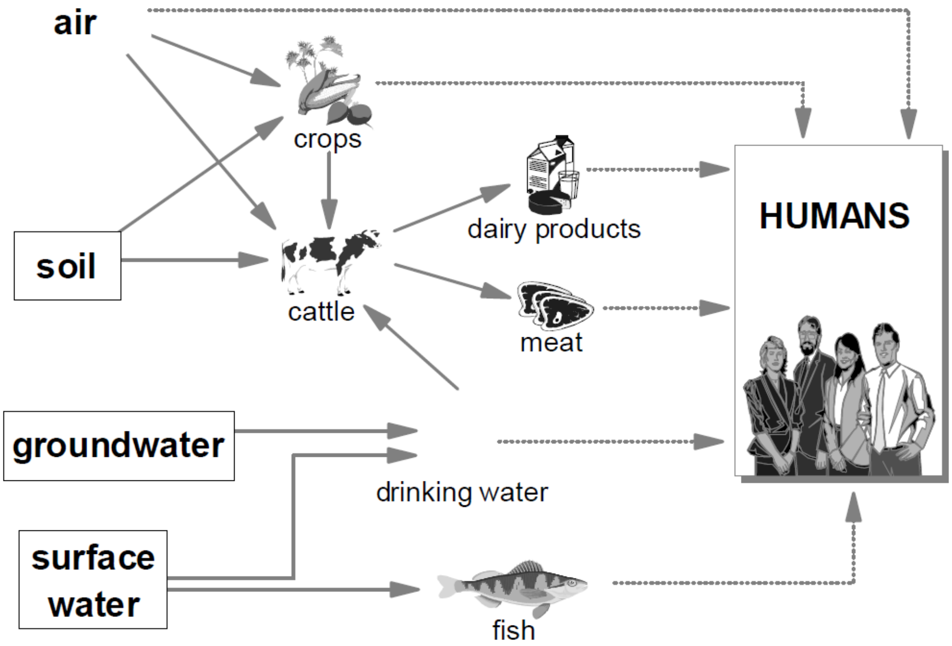


Figure 8: Indirect exposure routes for humans through the environment. Solid lines indicate (bio)transfer, broken lines indicate human intake.

The concentration of a substance in food is estimated from the concentration in water, soil and air taking into account the bioconcentration or bioaccumulation behaviour for the specific food items. The estimation of most bioconcentration factors (BCF) or bioaccumulation factors (BAF) is highly dependent on Kow. The estimations in EUSES are therefore only valid for organic, non-ionized or non-dissociating chemicals.

This section will not take metals into account since uptake and bioaccumulation are highly non-linear and metal-specific, hence beyond the scope of this section. Update needs and possible solutions for metals will be treated in separate sections (see topic 17).

17.2. Change proposed (why and what)

Plant leaves: In EUSES, uptake to leaves from soil water is calculated using the transpiration stream concentration factor (TSCF) based on Briggs et al. (1982), which is the quotient between the chemical concentrations in the transpiration stream and the soil pore water. This estimation of TSCF was derived for a small group of pesticides and one plant species (Barley). Ranging in log Kow from -0.5 to 4.5 (outside this range the minimum or maximum Kow is used in EUSES).

$$TSCF = 0.784 \cdot \exp\left[\frac{-(\log Kow - 1.78)^2}{2.44}\right]$$

Based on the work of Dettenmaier et al. (2009), this equation should be modified. They re-evaluated the relationship between root uptake and chemical hydrophobicity. In their study TSCFs were measured for 25 organic chemicals ranging in log Kow from-0.8 to 5. Using the TSCF values measured, a new empirical relationship between TSCF (0 and 1) and log Kow (-0.8 to 5) is presented that indicates that non-ionizable, polar, highly water soluble organic compounds are most likely to be taken up by plant roots and translocated to shoot tissue. Based on this work, the equation should be modified to:

$$\mathrm{TSCF} = \frac{11}{11 + 2.6^{\log K_{ow}}}$$

Compared to EUSES, a higher uptake in plant leaves is predicted for hydrophilic compounds.

Root crops: A validation study showed that EUSES severely overestimates root concentrations, due to the effect of growth dilution (Legind and Trapp, 2009). Because this is recognized also in the REACH Guidance (Chapter R7.10.10), EUSES should be updated. An updated model (Trapp, 2002) is recommended for the calculation of the concentration of neutral hydrophylics in roots from the concentration in soil water (Legind and Trapp 2009), as discussed by Franco et al. (p. 40-41).

In EUSES the general partitioning between water and plant tissue is assumed to be based on hydrophobic sorption to plant lipids. For hydrophilic chemicals the partition coefficient between plant tissue and water is calculated as

$K_{plant\text{-}water}$ = $Fwater_{plant}$ + $Flipid_{plant}$ x Kow^{b}

Where the default values for the plant parameters are:

$Fwater_{plant}$: 0.65

$Flipid_{plant}$: 0.01

b: 0.95

The concentration in root tissue is governed mainly by physical sorption, and is given by:

$$C_{root} = \frac{K_{plant\text{-}water} \cdot C_{agric,porew}}{RHO_{plant}}$$

The updated model available from Trapp (2002) uses a parameterization and root specific charactistics that are different from EUSES.

$$C_{\mathrm{R}} = \frac{Q}{Q/K_{\mathrm{RW}} + kV} C_{\mathrm{S}}$$

Where:

Q is the transpiration stream

k first order rate constant, the sum of an exponential growth rate and rate of metabolism, k_m

V is the root volume

Cs is the soil concentration

K_{RW} is the root water partition coefficient

The root volume and the first order rate constant are new parameters for which default parameters are provided by Trapp (2002). Growth dilution rate is set at 0.1 per day. Knowledge on metabolism rates inside the plants can be used, if available. The transpiration stream is the same as in EUSES.

The root water partition coefficient that is used subsequently differs in units and parameterization from EUSES and is

$$K_{\mathrm{RW}} = W + LaK_{\mathrm{ow}}^{b}$$

Where:

W is the root water fraction (0.89)

L is the root lipid content (0.025)

a density correction (1.22)

b empirical factor (0.77)

The proposed model approach is strictly limited to nonionizing and lipophilic compounds. It is not applicable to polar compounds and weak acids and electrolytes.

Meat and milk: The current regression equations in EUSES for estimating the biotransfer factors (BTFs) are based on Travis and Arms (1988):

$$BTF_{meat} = 10^{-7.6 + \log Kow} \quad (\log K_{OW} \text{ range } 1.5 \text{ to } 6.5)$$

$$BTF_{milk} = 10^{-8.1 + \log Kow} \quad (\log K_{OW} \text{ range } 3 \text{ to } 6.5)$$

The equations could be replaced by a mechanistic steady state model for bioaccumulation in cattle. The OSIRIS model (Franco et al., 2011) is based on McLachlan, 1994. From this mechanistic model concentrations in beef and milk are calculated with a default parameterization. The rather elaborate equations are given in Franco et al. (2011) including a list of default parameter values that could be employed. Applying these default parameter values, the equations only require standard EUSES input. Metabolic transfer rates can be and optionally used as input.

The comparison of the EUSES and OSIRIS models yielded considerable differences in human exposure via meat and dairy products. The differences were particularly large for (but by no means limited to) chemicals subject to biotransformation, as the EUSES model does not consider this possibility, while the OSIRIS model does.

For cattle fairly constant (and higher than EUSES) BAFs for persistent chemicals are predicted in the log Kow range of 3-6. The BAF values then drop at higher Kow (i.e. where EUSES BAFs are at maximum value). The octanol-air partitioning coefficient (Koa) is needed as input but can be obtained as Koa=Kow/Kaw, from standard input. The output in EUSES does not change. The model may need to be parameterized to represent a generic steer or cow by default. Due to the fact that different biotic compartments are involved in calculating BAFs, both soluble and lipophilic compounds are affected.

In the recommended mechanistic model, the metabolic rate constant is given as model input, enabling this model to capture the lower accumulation of labile compounds. When this rate constant is unknown, the most conservative approach is to assume that chemicals are not metabolized (Metabolism rate constant=0) as proposed by Franco et al. (2011).

The relationship between BAF or BTF and Kow in the OSIRIS model is consistent with experimental observations for persistent chemicals, while the Travis and Arms model is not (McLachlan, 1994; Hendriks et al., 2007).

17.3. Support for implementation

OSIRIS ITS-tool, available at http://osiris.simpple.com/OSIRIS-ITS/itstool.do

17.4. Priority level

Plant leaves

Criteria for priority evaluation:

1. Chemicals affected: A large number of chemicals is affected, both hydrophilic and lipophilic
2. Expected impact on exposure and/or alternative solutions available: Expected to be relatively low. Higher uptake anticipated compared to EUSES.

3. Maturity of the improvement (e.g. scientifically documented/ further research needed): Method is documented and validated.
4. Implementation in IT tools: implemented in the OSIRIS ITS-tool
5. Regulatory considerations: no
6. New data requirement? no

Suggested priority: Ready/ Important

The proposed method is ready to be implemented. Updating EUSES with this method is important because it predicts a higher uptake by plant leaves compared to EUSES. This affects exposure of man indirectly via the environment through the intake of food. The proposed method is only valid for neutral organic compounds, which is within in the current scope of EUSES.

Root crops

Criteria for priority evaluation:

1. Chemicals affected: A large number of chemicals is affected, both hydrophilic and lipophilic.
2. Expected impact on exposure and/or alternative solutions available: Expected to be relatively low. Root concentrations will be lower compared to EUSES.
3. Maturity of the improvement (e.g. scientifically documented/ further research needed): Method is documented and tested
4. Implementation in IT tools: implemented in the OSIRIS ITS-tool
5. Regulatory considerations: no
6. New data requirement? The new approach does not need more chemical data than except that knowledge about metabolism rates inside the plants can be used, if available.

Suggested priority: Ready/Important

EUSES severely overestimates root concentrations, due to the effect of growth dilution and therefore updating EUSES is important. An updated model for neutral hydrophobic chemicals is available from Trapp (2002). The proposed method is ready to be implemented. Updating EUSES with this method is important because it predicts lower uptake for root compared to EUSES. This affects exposure of man indirectly via the environment through the intake of food. The proposed method is only valid for neutral organic compounds, which is within in the current scope of EUSES.

Meat and Milk

Criteria for priority evaluation:

1. Chemicals affected: A large number of chemicals is affected, both hydrophilic and lipophilic especially those with high Kow (>6) values and those that potentially metabolize.
2. Expected impact on exposure and/or alternative solutions available: Expected to be relatively low.
3. Maturity of the improvement (e.g. scientifically documented/ further research needed): Method is documented model is consistent with observations
4. Implementation in IT tools: implemented in the OSIRIS ITS-tool
5. Regulatory considerations: No
6. New data requirement? Not necessary but metabolization rate constants can be used as input and Koa can be calculated from standard EUSES input

Suggested priority: Ready/Important

The OSIRIS model (based on McLachlan, 1994) is mechanistically based in contrast to the regression based BTF factors in EUSES. The two models also differ in their treatment of labile chemicals. The EUSES model assumes that Kow is the only chemical determinant of the BTF/BAF while the OSIRIS model assumes that biotransformation plays an important role and (optionally) incorporates this into the model equations. The proposed method is ready to be implemented. Updating EUSES with this method is important because it predicts a different bioaccumulation behavior (f.i. decrease in bioaccumulation at higher Kow values) compared to EUSES. This affects exposure of man indirectly via the environment through the intake of food.

As a general remark it is recognized that indirect human exposure is not often critical for the risk assessment (Bodar et al, 2003). The proposed update needs are valid for neutral organic compounds, which is within in the current scope of EUSES.

17.5. References

Bodar CWM, Berthault F, De Bruijn JHM, Van Leeuwen CJ, Pronk MEJ, T G Vermeire TG (2003). Evaluation of EU risk assessments existing chemicals (EC Regulation 793/93).Chemosphere 53(8):1039-47

Briggs G, Bromilow RH, Evans AA (1982). Relationships between lipophilicity and root uptake and translocation of nonionized chemicals by barley. Pesticide Science 13: 495-504.

Dettenmaier EM, Doucette WJ, Bugbee B (2009). Chemical Hydrophobicity and Uptake by Plant Roots. Environ. Sci. Technol. 43: 324-329.

ECHA (2012). Guidance on information requirements and chemical safety assessment. Chapter R.16: Environmental Exposure Estimation. Report ECHA-10-G-06-EN, Helsinki, Finland.

Franco A et al. (2011) OSIRIS Deliverable D3.1.17 (6th Framework Program, EU, Project no. 037017) Recommendations for adaptations of ECHA Guidance Documents and EUSES.

Hendriks AJ, Smitkova H, Huijbregts MAJ. A new twist on an old regression: Transfer of chemicals to beef and milk in human and ecological risk assessment. Chemosphere 2007; 70:

46-56.

Legind CN and Trapp S. (2009). Modeling the exposure of children and adults via diet to chemicals in the environment with crop-specific models. Environ. Pollut. 157: 778-785.

McLachlan MS (1994). Model of the Fate of Hydrophobic Contaminants in Cows. Environ. Sci. Technol. 1994; 28: 2407-2414.

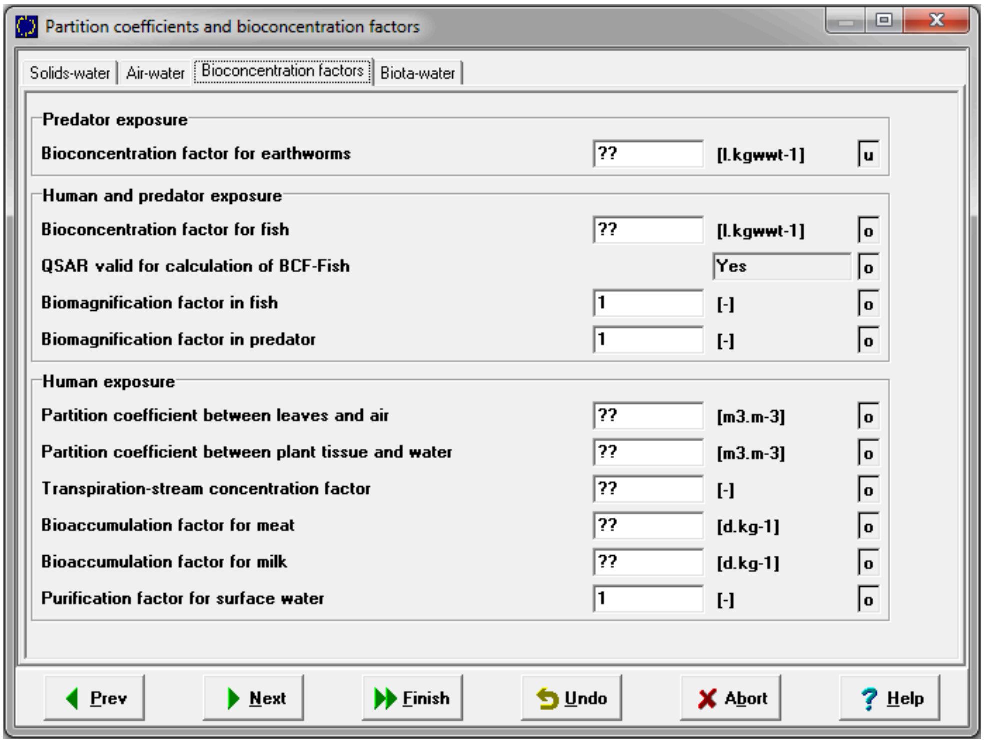
Trapp (2002). Dynamic Root Uptake Model for Neutral Lipophilic Organics. Environmental Toxicology and Chemistry, Vol. 21, No. 1, pp. 203–206.

Travis CC and Arms AD (1988). Bioconcentration of organics in beef, milk, and vegetation. Environ. Sci. Technol. 22, 271-274.

18. Man via the environment: alternative model for crop exposure pathway

18.1. Current situation in EUSES

In the current version of EUSES, several MvE fate parameters are estimated based on Log Kow and vapour pressure. Following parameters can be inputted:



Predator exposure

Bioconcentration factor for earthworms	??	[l.kgwwt-1]	u

Human and predator exposure

Bioconcentration factor for fish	??	[l.kgwwt-1]	o
QSAR valid for calculation of BCF-Fish		Yes	o
Biomagnification factor in fish	1	[-]	o
Biomagnification factor in predator	1	[-]	o

Human exposure

Partition coefficient between leaves and air	??	[m3.m-3]	o
Partition coefficient between plant tissue and water	??	[m3.m-3]	o
Transpiration-stream concentration factor	??	[-]	o
Bioaccumulation factor for meat	??	[d.kg-1]	o
Bioaccumulation factor for milk	??	[d.kg-1]	o
Purification factor for surface water	1	[-]	o

18.2. Change proposed (what)

Two changes are proposed regarding all crop related exposure pathways. Note that all other exposure pathways for man via the environment (i.e. meat and milk bioaccumulation routes, fish bioconcentration route, drinking water route, air inhalation route) can remain as they are.

1. Change in input interface

For inorganics, following fate parameters are not always valid because they are based on log Kow and vapour pressure:

- Partition coefficient between leaves and air
- Partition coefficient between plant tissue and water
- Transpiration-stream concentration factor

For inorganics, these parameters cannot be estimated with current equations based on log Kow and vapour pressure. Also, alternative, available data on crop transfer is typically expressed in different units (as mass basis instead of volume basis). Instead, an user should be able to input following three additional/alternative parameters:

$\boldsymbol{TF_{roots,soil}}$ is the dwt transfer factor from soil to roots (expressed in $kg_{soil}.kg_{roots}^{-1}$)

$\boldsymbol{TF_{leaves,soil}}$ is the dwt transfer factor from soil to leaves (expressed in $kg_{soil}.kg_{leaves}^{-1}$)

$\boldsymbol{TF_{grass,soil}}$ is the dwt transfer factor from soil to grass (expressed in $kg_{soil}.kg_{grass}^{-1}$)

Practically, an user should select whether the man via the environment calculations are to done according to the “lipophilicity based” equations (default setting) or according to the alternative equations in next section.

2. Separate calculations for inorganics

The current lipophicilicity based modelling approach proposed by Trapp and Matthies (1995) is used to estimate levels in plants due to uptake from pore water and air (gas phase). This approach integrates uptake from pore water and air into a consistent, one-compartment model. The sink term in the model is formed by diffusive transfer from leaf to air, elimination in the plant tissue, and dilution by growth; the source term is formed by the uptake and translocation from soil and gaseous uptake from air. Aerosol deposition is not considered in the model. The general partitioning between water and plant tissue is assumed to be based on hydrophobic sorption to plant lipids. *Kow* is corrected slightly for the differences between plant lipids and octanol. The concentration in root tissue is governed mainly by physical sorption. The transpiration-stream concentration factor (*TSCF*) is the ratio between the concentration in the transpiration stream and the concentration in pore water. *TSCF* is given by (Briggs *et al.*, 1982). This estimation of *TSCF* was derived for a small group of pesticides in one plant species (Barley). Domain of physico-chemical properties: log *Kow* -0.5 to 4.5 (outside this range the minimum or maximum *Kow* is used). Gaseous exchange between leaves and air can be described by a leaf-air partition coefficient. Elimination of the substance may take place in the leaf tissue by metabolism or photolysis.

For inorganics, a comprehensive approach is considered by considering measured data for transfer factors from soil to root, leaves and grass. This leads to simplified model calculations:

$$\boldsymbol{C_{roots}} = \boldsymbol{TF_{roots,soil}} \cdot \boldsymbol{C_{soil}}$$

$$\boldsymbol{C_{leaves}} = \boldsymbol{TF_{leaves,soil}} \cdot \boldsymbol{C_{soil}}$$

$$\boldsymbol{C_{grass}} = \boldsymbol{TF_{grass,soil}} \cdot \boldsymbol{C_{soil}}$$

with

$\boldsymbol{C_{soil}}$ is the dwt concentration in soil, expressed in $kg.kg_{soil}^{-1}$

$C_{root/leaves/grass\ (wwt)} = C_{root/leaves/grass\ (dwt)}$ x $(1- Fwater_{plant})$

The water content (ca. 93 %w/w) in crops ($Fwater_{plant}$) can be calculated using existing EUSES defaults (volume fraction of water in plant tissue (65% %v/v) and the bulk density of plant tissue (0.7 kg/L)).

18.3. Why to propose such change

MvE EUSES calculations are currently not valid for metals and therefore it is not relevant to apply them for metals. MvE assessment can be one of the key drivers in REACH Authorizations population impact calculations.

18.4. Input and output

See section 17.2. Transfer factors for inorganics can be obtained from literature (human health and environmental sciences, agricultural sciences and environmental technology (phytoremediation)). Guidance would need to be developed to assess the relevancy and quality of measured transfer factors. Following criteria could for example be considered:

- Only transfer factors originating from field data (incl. urban gardens) or laboratory studies using soil and biota collected at the same field site should been retained (small pot trials or greenhouse experiments can be excluded); this is to ensure that biota burdens are in equilibrium with soil concentrations.
- Only transfer factors for edible, mature crops or crop parts should be considered (to maintain relevance for human consumption);
- Transfer factors from soils with freshly added metal salts should be excluded because transfer of metals from freshly spiked soils might not be representative for transfer of metals from field contaminated soils. This is because metals in freshly spiked soils are more mobile than in field contaminated soils, where metals have undergone aging processes (*Efroymson et al., 2007; Smolders et al., 2009*).
- Steady-state equilibrium must be reached in case of coupled data (in soil and food matrices). Crops are preferably sampled just before harvest.
- Only relevant soil concentrations are considered (highly polluted soils are to be excluded)

Note that there are currently no entries foreseen in IUCLID for all MvE fate parameters (i.e. the parameters discussed here and bioaccumulation for meat and milk).

18.5. Support for implementation

- > 50 Publications describing the definition of transfer factor (key publication not identified so far)
- No specific existing tools/excel spreadsheet due to simplicity of equations. Some models already include the possibility to use transfer factors as input for the risk assessment.

18.6. Priority level

1. Number (type of) of chemicals affected: low (metals/inorganics) but high tonnage chemicals with high need under REACH Authorization process
2. Maturity: Scientifically documented: yes
3. Implemented into IT tool : not relevant due to simplicity of equations
4. Regulatory considerations : high need under REACH authorization process.
5. Expected impact on exposure: be able to calculate MvE exposure for inorganics (not possible with current EUSES version).
6. New data requirement: Yes but only for type of chemicals affected, transfer factors from soil to root, leaves and grass.

Suggested priority: Ready/high importance for metals/inorganics

19. Secondary poisoning

19.1. Current situation in EUSES

In EUSES three food chains are considered:

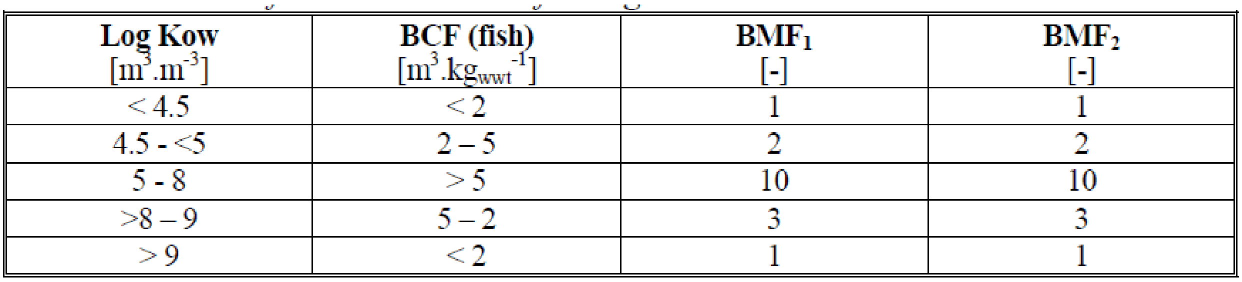
- Water (freshwater and marine environment) => fish => fish-eating predator.
- Water (marine environment) => fish => fish-eating predator => top-predator;
- Soil => earthworm => worm-eating predator.

These three food chains are examples of secondary poisoning pathways. However, safe levels for fish-eating animals do not exclude the possibility of risks to other birds or mammals feeding on other aquatic organisms (e.g. mussels and worms). It is therefore emphasized that the proposed methodology merely gives an indication that secondary poisoning is a critical process in the aquatic risk characterization of a chemical.

The concentrations in food (fish and earthworms) are calculated from the concentration in the environment (surface water and agricultural soil) and the measured or estimated BCFs (see chapter 1). For the freshwater and marine environment also a biomagnification factor (BMF) must be applied.

To go up the food chain from a small fish to a predatory fish BMFs are needed additionally.

Default values for BMFs for different log Kow-ranges are also provided. The BMF can either be based on the available log Kow or BCF:



Log Kow $[m^3.m^{-3}]$	BCF (fish) $[m^3.kg_{wwt}^{-1}]$	BMF_1 [-]	BMF_2 [-]
< 4.5	< 2	1	1
4.5 - <5	2 – 5	2	2
5 - 8	> 5	10	10
>8 – 9	5 – 2	3	3
> 9	< 2	1	1

Concentration in fish:

Cfish = BCFfish * Cwater

Fish eating predators:

PECoral,fish = Cwater * BCFfish * BMF1

Fish-eating top predators:

PECoral,fish = Cwater * BCFfish * BMF1 * BMF2

With respect to man indirectly exposure via the environment it has to be noted that biomagnification in the fish food chain (i.e., accounting for the fact that predatory fish are consumed as well) is not taken into account in the calculations for fish consumed by humans in EUSES. The addition of predatory fish in the aquatic food chain in order to account for biomagnification could be considered indirect human exposure assessment.

19.2. Change proposed (why and what)

Modifying aquatic food chain:

Franco et al. (2011, OSIRIS model) suggested an improved model for a piscivorous fish feeding exclusively on a planktivorous fish. The fish sub-model has a default parameterization that was based on the zooplankton – herring – cod food chain in the Baltic Sea.

Therefore, two fish concentrations are reported: in a fish feeding on zooplankton and a predatory fish feeding on planktivorous fish. The current EUSES model only considers the first fish trophic level as food source where the potential biomagnification of (highly) lipophilic substances in the next trophic level for fish is ignored. Additionally EUSES does not consider that feeding on plankton can also contribute to bioaccumulation next to direct exposure to dissolved chemicals in water.

OSIRIS proposal:

Water => plankton => fish => piscivorous fish

However they made no clear proposal how this food chain should be implemented in the existing EUSES food chains. It could either be treated as a new separate food chain or the piscivorous fish could serve as a food source for fish-eating predators (birds and mammals). The latter would result in an extra level in the existing aquatic food chain as implemented in EUSES:

- Water (marine and fresh) => fish => piscivorous fish => fish-eating predator.
- Water (marine) => fish => piscivorous fish => fish-eating predator => top-predator;

Addition a terrestrial food chain:

Addition of a new terrestrial food chain in analogy with the aquatic food chain is advocated, as an extension to the current protection targets with the same number of trophic levels as the aquatic food promoting consistency in the risk assessment for secondary poisoning:

Soil => earthworm => worm-eating predator => top-predator

The methodology is straightforward and comparable with the aquatic food chain. It is recognized that protocols for terrestrial bioaccumulation assessments are far less-developed than for aquatic systems (Gobas, 2015). Additional biomagnification factors are required for terrestrial top-predactors, which are not available in EUSES. These may be derived from Verbruggen (2014) but further research is needed on the availability of empirical BMF–Kow relationships or QSAR models. Model output is extended with a risk characterization for terrestrial top predators

19.3. Priority level

Modification of aquatic food chain:

Criteria for priority evaluation:

1. Chemicals affected: A sizeable number of particularly neutral organic chemicals potentially bioaccumulating, having a log Kow > 5.
2. Expected impact on exposure and/or alternative solutions available: The impact for bioaccumulating substances may be relatively high, due to additional bioaccumulation that is modelled in newly proposed aquatic food chains..
3. Maturity of the improvement (e.g. scientifically documented/ further research needed): Method is scientifically documented. Sub-model or process is verified. The Franco model is verified on PCBs. The implementation of the addition of piscivorous fish to the existing aquatic food chains in EUSES needs some consideration.
4. Implementation in IT tools: no
5. Regulatory considerations: no
6. New data requirement? Additional biomagnification factors are required for piscivorous fish..

<u>Suggested priority:</u> Not ready (needs further research)/medium importance

Biomagnification in the fish food chain accounting for the fact that predatory fish are consumed as well (going up the food chain from a small fish to a predatory fish) is not taken into account in EUSES. This might as well be relevant for human indirectly exposed via the environment taking into account that predatory fish are consumed by humans.

There are two options on how the modification of the aquatic food chain should be implemented in EUSES, either as a new separate food chain or the piscivorous fish could serve as a food source for fish-eating predators (birds and mammals). The latter would result in an extra level in the existing aquatic food chains in EUSES.

The impact for bioaccumulating substances may be relatively high, due to additional bioaccumulation that is modelled in the food chains for a sizeable number of neutral organic chemicals.

In principle, all substances that undergo an assessment for secondary poisoning are affected due to the changes implemented, but on a general note, bioaccumulation is mostly of concern for substances with a log Kow value > 5.

Additional terrestrial food chain:

Criteria for priority evaluation:

1. Chemicals affected: all types of chemicals (type, number): Sizeable; affects chemicals with bioaccumulation potential with log Kow > 4.
2. Expected impact on exposure and/or alternative solutions available: The impact of these equations is expected to be relatively high for bioaccumulating substances.
3. Maturity of the improvement (e.g. scientifically documented/ further research needed): Biomagnification factors for top-predators are needed but have not been specified yet. Further research is needed on the availability of empirical BMF–Kow relationships or QSAR models. The methodology is straightforward and comparable with the aquatic food chain. Although it is recognised that protocols for terrestrial bioaccumulation assessments are far less-developed than for aquatic systems.
4. Implementation in IT tools:
5. Regulatory considerations: A consistent set of protection targets for secondary poisoning may be considered when revising the relevant guidance.
6. New data requirement? Biomagnification factors for terrestrial top-predators

Suggested priority: Not ready (needs further analysis on implementation)/high importance

Proposed method is rather straight forward by itself, mainly suggested for the reason of consistency but not fully ready to implement in EUSES. Biomagnification factors are required though but have not yet been specified. Additional research is needed on the availability of empirical BMF–Kow relationships or QSAR models. Furthermore a consistent set of protection targets for secondary poisoning may be needed to be implemented first in the relevant guidance.

Addition of a new food chain in analogy with the aquatic food chain is advocated, as an extension to the current protection targets with the same number of trophic levels as the aquatic food chain. Additional biomagnification factors are required though for terrestrial top-predators and are not available in EUSES. Model output is extended with a risk characterisation for terrestrial top predators. The impact of these equations is expected to be relatively high for bioaccumulating substances due to additional bioaccumulation in the modelled food chain.

19.4. References

Arnot JA, Mackay D, Parkerton TF, Zaleski RT, Warren CS (2010). Multimedia modelling of human exposure to chemical substances: the roles of food web biomagnification and biotransformation. Environ Toxicol Chem 29: 45-55.

ECHA (2014). Guidance on Information Requirements and Chemical Safety Assessment Chapter R.11: PBT/vPvB Assessment. Report ECHA-14-G-07-EN, Helsinki Finland.

Environment UK (1999). Review of bioaccumulation models for use in environmental standards Science Report – SC030197/SR1.

Franco A et al., (2011) OSIRIS Deliverable D3.1.17 (6th Framework Program, EU, Project no. 037017) Recommendations for adaptations of ECHA Guidance Documents and EUSES.

Gobas FAPC, Burkhard LF, Doucette WJ, Sappington KG, Verbruggen EMJ et al al (2015) Review of Existing Terrestrial Bioaccumulation Models and Terrestrial Bioaccumulation Modeling Needs for Organic Chemicals. Integrated Environmental Assessment and Management — Volume 12, Number 1—pp. 123–134

Kelly BC, Ikonomou MG, Blair JD, Surridge B, Hoover D, Grace R, Gobas FA (2009) Perfluoroalkyl contaminants in an Arctic marine food web: trophic magnification and wildlife exposure. Environ Sci Technol. 43(11):4037-4043

Rorije E, Verbruggen EAJ, Hollander A, Traas TP, Janssen MPM (2011). Identifying potential POP and PBT substances. Development of a new Persistence/Bioaccumulation-score, RIVM Report 601356001/2011, Bilthoven the Netherlands.

20. Nanomaterials (chemicals in solid state / particulates)

20.1. Current situation in EUSES

The standard EUSES approach, described in the TGD cannot adequately model the environmental fate and exposure of engineered nanomaterials due to fundamental differences between behaviour of ‘dissolved’ and particulate chemicals (Meesters et al. 2013). Multi-compartmental box models such as the SimpleBox model basically assume first order transport and transformation processes for dissolved chemicals. This also applies to nanomaterials, but the underlying mechanisms affecting nanomaterial transport and transformation differ and need to be added.

In relation to conventional chemicals, engineered nanomaterials (ENMs) are of a particulate nature, meaning that they are not dissolved in solution but exist as two distinct phases (E.g. solid and liquid) which are thermodynamically unstable. For this reason, the fate of ENMs cannot be defined by thermodynamic equilibrium coefficients for partitioning. However the tendency of ENMs to reach (a more) thermodynamic stable state still makes it possible to define rates for transformation and transport.

Currently the partitioning between media is parameterized based on partitioning coefficients, whereas for nanomaterials this is based on the affinity of nanomaterials to stick to other solids. Furthermore, the process is called a transformation process from free nanomaterials to hetero-aggregates containing nanomaterials, but based on the size fraction these can still be considered bioavailable.

20.2. Change proposed (why and what)

SimpleBox4.0-nano is an extension of the SimpleBox model, which is designed to simulate the specific environmental behaviour of nanomaterials in order to derive a predicted environmental concentration (PEC) for a nanomaterial. This will become relevant when specific information for nanomaterials is required for registration of chemicals in the EU.

The main adaptation consists of adding three particulate chemical species to the dissolved species already included in SimpleBox. SimpleBox4.0-nano calculates mass flows of nanomaterials by simultaneously solving mass balance equations for four different chemical species for each environmental compartment in the model (Figure 9). Although four different chemical species are calculated, in terms of deriving PECs for risk assessment, these can be reduced to two species: the dissolved chemical and the total nanomaterial concentration.

The modifications to extend EUSES for use with nanomaterials would include the adaptation of transport processes that are dependent on particle size for wet and dry deposition from air to soil and water, and sedimentation from water to sediment. Because of this size dependence the process of agglomeration of nanomaterials with larger natural particles affects their fate. Furthermore dissolution, mainly of metal or metal oxide nanomaterials plays an important role. Several other processes are similar for other chemical groups such as degradation, but might require novel methods for measuring their rate constants.

This change adds more chemical species, e.g. the particulate form to the current model. This results in the extension of the calculation matrix in order to accommodate the three additional chemical species. The main input parameters consist of characteristics of the nanomaterial, the attachment efficiency or heteroagglomeration rate constant between nanomaterial and natural particles, and the dissolution rate constant of the nanomaterial. These can be specified based on the environmental compartment.

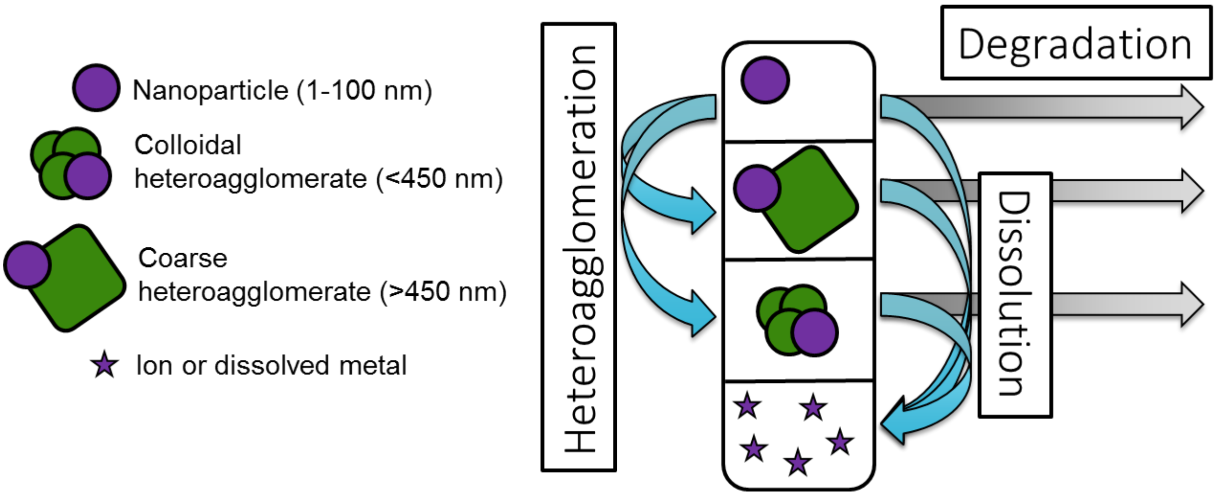


Figure 9: Overview of the four different chemical species and the nanoparticle transformation processes incorporated in the calculation matrix of SimpleBox4.0-nano.

20.3. Support for implementation

The definition of the fit for nanomaterials multimedia fate model extension was published in 2014 (Meesters et al. 2014). Since then the model has been tested and reviewed (Jacobs et al. 2016; Meesters et al. 2016; Nowack 2017; Quik 2018) and its function highlighted in risk assessment of nanomaterials. Furthermore the model has shown its use in life cycle impact assessment of nanomaterials (Ettrup et al. 2017; Pini 2016; Salieri 2018). Since 2016 the model definition by Meesters et al. (2014) as incorporated into SimpleBox4.0 has been made available as spreadsheet from the RIVM website [link] and downloaded over 100 times. Within the EU projects NanoFASE and CaLIBRAte work is continuing on developing the SimpleBox4nano model. Within the OECD a new test guideline (TG 318) on dispersion stability of nanomaterials has been published (OECD, 2017) and a new test guideline on dissolution rate of nanomaterials is under preparation. On top of these two test guidelines a Guidance Document is under preparation to describe the linkages between the two test guidelines, which also pays attention to the application of these two OECD test guidelines in measuring input parameters for fate modelling.

20.4. Priority level

Criteria for priority evaluation:

1. Chemicals affected: All chemicals in nanoform.
2. Expected impact on exposure and/or alternative solutions available: The proposed method is an extension of the applicability domain of the current EUSES version. It only covers the fate and distribution part at regional scale. Solutions for the other modules are not covered in the current proposal, i.e. emissions (the nano form will have to be distinguished), man indirectly exposed via the environment, secondary poisoning and risk characterisation.
3. Maturity of the improvement (e.g. scientifically documented/ further research needed): The provided modelling method for estimating predicted exposure concentrations of nanomaterials is scientifically documented. Further research is primarily required to identify the specific forms that need to be included in the PEC to provide a proper risk characterisation. It is expected that an updated SimpleBox4.0-nano version will be published at the end of the NanoFASE project.
4. Implementation in IT tools: SimpleBox4.0-nano spreadsheet version
5. Regulatory considerations: Currently, the REACH Annexes are being adapted for nanomaterials. These adaptations require that the chemical safety assessment shall address nanoforms that are covered by the registration, and specific requirements for nanoforms are indicated in the different Annexes. It is anticipated that these changes will enter into force by 1 January 2020.
6. New data requirement? Primarily physico-chemical characteristics of the nanomaterial are required as new input requirements, including the emission rate, the size, shape and

coating, heteroagglomeration rate or attachment efficiency, and the dissolution rate. The adapted REACH Annexes will require characterisation of the nanoforms by size (distribution), surface area, shape and surface chemistry (including coating, functionalisation, etc.). In addition, dissolution rate and dispersion stability will be required in Annex VII.

Suggested: Technically ready with respect to fate modelling of nanomaterials at regional scale. Not ready for implementation/ High importance

The proposed adaptation to extend EUSES for use with nanomaterials and particles in general is theoretically ready for implementation, although the link with other modules needs to be taken into consideration. It is an important extension of the current applicability domain of EUSES towards nanomaterials. Furthermore the proposed modelling approach will facilitate improvements in modelling of other chemical groups as well, e.g. inclusion of different metal species (dissolved vs solid particles), or application for modelling the fate of larger particles such as microplastics.

20.5. References

Salieri, B., R. Hischier, J. T. K. Quik and O. Jolliet. 2018. "Fate modelling of nanoparticle release in LCA: An integrative approach towards "USEtox4Nano"." Submitted.

Ettrup, K., A. Kounina, S. F. Hansen, J. A. Meesters, E. B. Vea, and A. Laurent. 2017. 'Development of Comparative Toxicity Potentials of TiO2 Nanoparticles for Use in Life Cycle Assessment', Environ Sci Technol, 51: 4027-37.

Jacobs, R., J. A. Meesters, C. J. Ter Braak, D. van de Meent, and H. van der Voet. 2016. 'Combining exposure and effect modeling into an integrated probabilistic environmental risk assessment for nanoparticles', Environ Toxicol Chem, 35: 2958-67.

Koelmans, A. A., N. J. Diepens, I. Velzeboer, E. Besseling, J. T. Quik, and D. van de Meent. 2015. 'Guidance for the prognostic risk assessment of nanomaterials in aquatic ecosystems', Sci Total Environ, 535: 141-9.

Meesters, J. A. J., A. A. Koelmans, J. T. Quik, A. J. Hendriks, and D. van de Meent. 2014. 'Multimedia modeling of engineered nanoparticles with SimpleBox4nano: model definition and evaluation', Environ Sci Technol, 48: 5726-36.

Meesters, J. A. J., J. T. K. Quik, A. A. Koelmans, A. J. Hendriks, and D. van de Meent. 2016. 'Multimedia environmental fate and speciation of engineered nanoparticles: a probabilistic modeling approach', Environ. Sci.: Nano, 3: 715-27.

Meesters, J. A., K. Veltman, A. J. Hendriks, and D. van de Meent. 2013. 'Environmental exposure assessment of engineered nanoparticles: why REACH needs adjustment', Integr Environ Assess Manag, 9: e15-26.

Nowack, Bernd. 2017. 'Evaluation of environmental exposure models for engineered nanomaterials in a regulatory context', NanoImpact, 8: 38-47.

OECD. 2017. Test No. 318: Dispersion Stability of Nanomaterials in Simulated Environmental Media, OECD Guidelines for the Testing of Chemicals, Section 3, No. 318, OECD Publishing, Paris, http://dx.doi.org/10.1787/9789264284142-en

Pini, M., B. Salieri, A. M. Ferrari, B. Nowack and R. Hischier. 2016. "Human health characterization factors of nano-TiO2 for indoor and outdoor environments." The International Journal of Life Cycle Assessment 21(10): 1452-1462.

21. Release and fate of sparingly soluble chemicals

21.1. Current situation in EUSES

Many sparingly soluble chemicals (e.g. most metal oxides, many metal salts, some organic substances) are released to the environment in pure solid or liquid forms that are not readily transformed into the environmentally active (dissolved) form. Currently EUSES does not distinguish between physical forms in which chemical substances may occur, or in which form they are released, thereby silently assuming that chemicals appear entirely in the dissolved form, at least instantaneously upon release in the environment.

Current approaches for estimating the release include the use of SPERCs or measured effluent data that usually consider both the pure solid particles and dissolved forms (unless samples are filtered before analysis). This is a worst-case approach as solid particles are assumed to be transformed into the environmentally active (dissolved) form once emitted to the aquatic compartment.

21.2. Change proposed (what)

This can be improved by modelling the process of dissolution at the local and regional scale in EUSES, as proposed by Meesters et al. (2013) and Farley et al. (2011). Instead of assuming instantaneous dissolution for all chemicals and silent disregard of the form in which the substance is released, EUSES could be modified to take account of (i) the form in which the substance is released, and (ii) estimate the rate of formation of the dissolved form as a first-order process, characterised by a first-order dissolution rate constant. Subsequently, the emission of solid physical form and dissolved physical form needs to be handled in the local and regional fate modelling as well. Further clarifications are needed on whether the dissolution kinetics should be explicitly considered in the release estimation or whether a dissolved fraction is to be calculated. It makes sense to consider the dissolution kinetics in the fate modelling. Further clarification is needed on how to model floating material (e.g. based on density). The most likely existing model that has considered different physical forms is Simplebox for nano. It needs to be assessed whether this model can also be applied for larger (than nano) particles (see separate topic).

Note that speciation and bio-availability of metals is not foreseen in this topic because part of another topic.

21.3. Why to propose such change

Otherwise, the current EUSES model may lead to serious overestimation of exposure concentrations (particularly so for metals in water), which is described well in the literature (Diamond et al., 2010). Slow solubility and its consequences for exposure estimation have also been described for nanomaterials.

The proposed change affects exposure concentrations (local and regional PECs) in water, sediment and biota, particularly for substances emitted in solid form to water. Accounting for slow dissolution could lead to lower predicted concentrations in water and higher concentrations in (the solid phases of) sediments or could lead to higher predicted concentrations in water, e.g. when chemicals will float on the surface water.

Accounting for slow dissolution requires that additional information is available: (i) registrants must specify the form in which the chemical is released, and (ii) in case the chemical is released as a solid, a first-order rate constant for dissolution must be provided. Such information can be obtained by laboratory testing according to TD protocol: OECD Guideline 29 (2001). The proposed change would result in more realistic PEC assessments; no new model output is expected (but to be further clarified).

21.4. Support for implementation

Implementation of the changes proposed to turn EUSES ‘fit for nano’, as described by Meesters et al., 2013 (section 19) would include accounting for slow dissolution of solids. Meesters’ model is a prototype, available for research purposes in spreadsheet format. Implementation of slow dissolution only would be a minor effort, compared to model adaptation necessary for nanomaterials.

21.5. Priority level

1. Number (type of) of chemicals affected: medium: all sparingly soluble chemicals
2. Maturity: documented: yes but several clarifications have to be made
3. Implemented into IT tool : no, however, SimpleBox for nano may contain valuable implementation given the comparable conceptual model design of considering particles and their dissolution
4. Regulatory considerations : no
5. Expected impact on exposure: The impact can be large.
6. New data requirement: +/- Yes, OECD 29 (7 days) for metals is not directly a testing requirement but can replace the water solubility endpoint for metals and metal compounds.

Suggested priority: Not ready/ low importance

21.6. References

Diamond ML, N Gandhi N, Adams WJ, Atherton J, Bhavsar SP, Bulle C, Campbell PGC, Dubreuil A, Fairbrother A, Farley K, Green A, Guinee J, Hauschild MZ, Huijbregts MAJ, Humbert S, Jensen KS, Jolliet O, Margni M, McGeer JC, Peijnenburg WJGM, Rosenbaum R, van de Meent D, Vijver MG (2010). The clearwater consensus: the estimation of metal hazard in fresh water. Int J Life Cycle Asses 15(2010), 143–147

Farley KJ, Carbonaro RF, Fanelli CJ, Costanzo R, Rader K, Di Toro (2011) TICKET-UWM: a coupled kinetic, equilibrium, and transport screening model for metals in lakes. Environmental Toxicology and Chemistry 30(6), 1278-1287.

Meesters JA, Veltman K, Hendriks AJ, van de Meent D (2013) Environmental exposure assessment of engineered nanoparticles: why REACH needs adjustment. Integrated environmental assessment and management 9(3):e15-26 doi:10.1002/ieam.1446

OECD (2001). Series on testing and assessment Number 29: Guidance document on transformation/dissolution of metals and metal compounds in aqueaous media. Paris. OECD document ENV/JM/MONO(2001)9.

22. Extended regional (and local) exposure modelling for metals

22.1. Current situation in EUSES

Current regional EUSES model is a Mackay level III model, it only allows to calculate steady-state PECs. EUSES has been developed primarily for organic substances (e.g. modelling of biodegradation) and needs extensions to predict the fate and exposure of metals. Metals do not biodegrade, instead they are subject to long term immobilization/mineralisation fate processes for metals which are currently not included in EUSES.

These long-term immobilization/mineralisation fate processes (like ageing) are currently considered as “correction factors” which are applied a posteriori to the PEC calculations outside the EUSES model.

22.2. Change proposed (what)

Option 1: Level IV Mackay model at regional scale (short term solution)

It should be allowed to calculate PECs after a surveyable time period (e.g. 100 years in case steady-state is not reached) or at least to give an indication when e.g. 95% of steady-state is reached. The spreadsheet version of SimpleBox already contains the option to perform dynamic Mackay level IV calculations, which allows to calculate regional PECs after a –to be defined- time period. It details how the calculations are expected to be carried out.

Option 2: Inclusion of additional, metal-specific fate processes at regional and, where relevant local scale (long term solution)

Currently, two models are available and described in the scientific literature that consider additional, metal-specific fate processes: for freshwater/sediment: TICKET-UWM (Farley et al., 2011)) and for soil (and subsequent freshwater/sediment) IDMM (Lofts et al., 2013). Some of the additional, metal-specific fate processes have already been added in USEtox (Ghandi) (but not all).

Following additional relevant fate processes for metals should be considered in the water and sediment compartment (Figure 10, Farley et al., 2011):

- metal binding to inorganic ligands, DOC (Dissolved Organic Carbon) and POC (Particulate Organic Carbon), hydrous ferric oxide (HFO) and hydrous manganese oxide (HMO); (partly implemented in USEtox)
- metal binding to biological receptors using information from the Biotic Ligand Model; (further discussed in other topic)
- metal precipitation as (hydr)oxides, carbonates and sulphides;
- dissolution kinetics for metal powders, massives, etc.; (further discussed in topic on “sparingly soluble chemicals”)
- average annual cycling of organic matter and sulphide production in the aquatic compartment;

These features allow better prediction of the fate, behaviour and risks of metals.

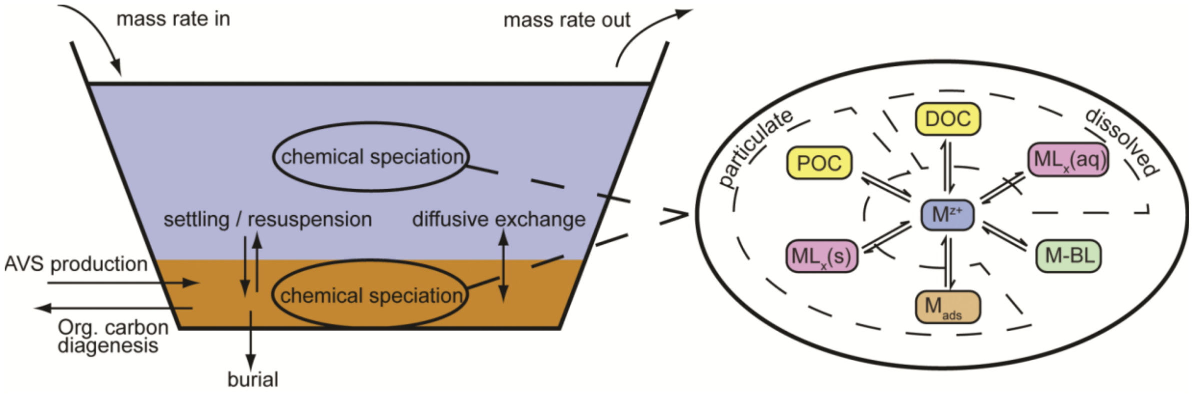


Figure 10: Conceptual model for the TICKET Unit World Model for Metals in Lakes (TICKET-UWM).

Following additional relevant fate processes for metals should be considered for the soil compartment (Lofts et al., 2013):

- three main forms of metal considered – labile, aged and mineral – represent the following species of metals:
    - labile metal represents metal dissolved in the porewater and metal adsorbed to the surfaces of fine soil;
    - aged metal represents metal ‘fixed’ into the fine soil solids. Metal transfer between the labile and aged forms is reversible and is modelled using first order kinetic expressions derived from laboratory studies of fixation;
    - mineral metal represents metal which is strongly fixed in the soil solids, for example metal derived from the parent material during soil formation. This pool supplies metal to the labile pool through weathering, which is described by first order kinetics. This pool is replenished by kinetically-modelled transfer of metal from the aged pool.

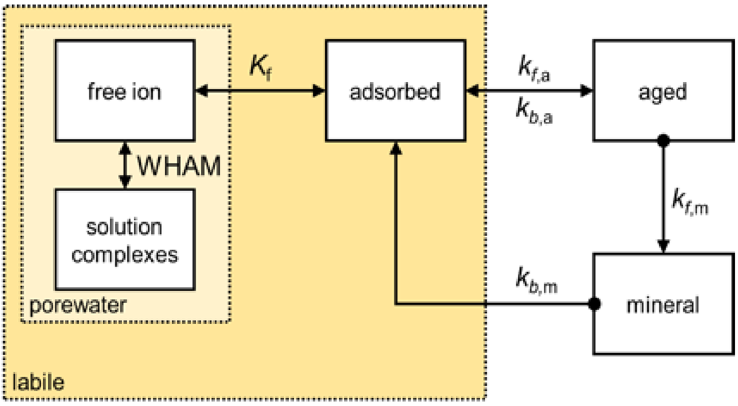


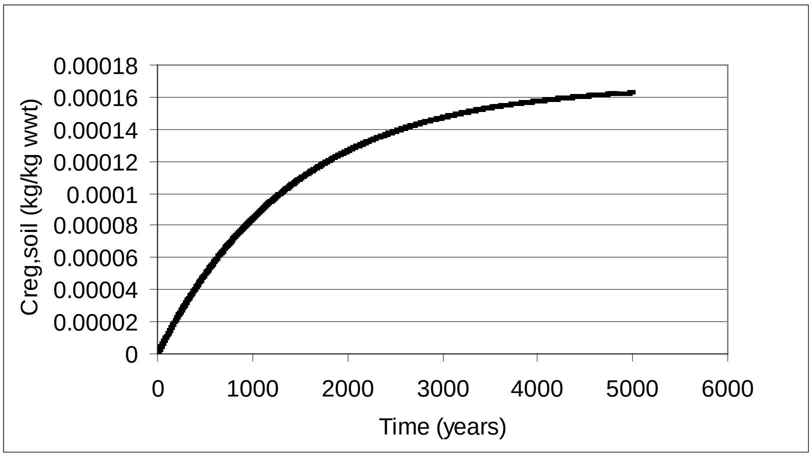
Figure 2. Schematic diagram of metal transformations in soils. Large K denotes an equilibrium transformation parameter, small k denotes a kinetic transformation parameter.

Detailed metal speciation modelling (cfr. WHAM) is currently not yet considered in this topic because it is part of another topic.

22.3. Why to propose such change

Despite the fact that measured data are often used for assessing the regional PEC for metals in the REACH registration process, the regional PEC modelling is relevant in case specific uses are to be assessed, like in the REACH authorization process. Measured data integrate all uses and historical contamination.

For metals, steady-state PEC regional in the soil and sediment compartment is in the current EUSES version only reached after hundreds or thousands of years (example: see figure below). This time frame is not relevant from a regulatory perspective. Under the ESR of Cd RAR, it is accepted (in the TM/TC-NES) to calculated PECs after reasonable time frames.



If the change is not implemented, PECregional is significantly overestimated for metals.

EUSES can only consider the use of metal-specific partition coefficients (Kp) instead of the octanol-water partition coefficient in the model. Sorption of metals is controlled not only by organic matter but by other solid-phase constituents like clay minerals and oxides. Moreover, the distribution of metals between the solid and liquid phase is not only controlled by pure adsorption/desorption mechanisms, but processes like precipitation or encapsulation in the mineral fraction also play a role. Environmental conditions (pH, redox conditions, temperature, ionic strength) and the composition of the liquid and solid phase have a strong effect on the Kp of inorganic substances. As a result, a wide range of Kp values have been reported and it is not always clear which value to select in a generic assessment.

EUSES modules affected is the regional exposure model (SimpleBox) in option 1 and option 2. In option 2, several fate processes are also relevant for consideration in the local exposure model.

22.4. Input and output

Option 1

Additional input: time point at which PECregional is to be calculated

Additional output: PECregional at the time point for all environmental compartments (sediment and soil being more relevant).

Option 2

Several additional inputs will be required. Additional outputs will be generated but if or which to be communicated: this needs to be further outlined. These outputs would give additional information on the truly dissolved fraction versus the adsorbed and immobilized fraction. It would not lead to additional protection targets.

22.5. Support for implementation

Option 1

- Regulatory acceptance in
    - Cd RAR page 287-291: https://echa.europa.eu/documents/10162/4ea8883d-bd43-45fb-86a3-14fa6fa9e6f3
    - ECHA Guidance Appendix R.7.13-2: environmental risk assessment for metals and metal compounds (https://echa.europa.eu/documents/10162/13632/information_requirements_r7_13_2_en.pdf)
- Tools/excel spreadsheets where the concept has been already implemented: Yes, Simplebox 2.0 spreadsheet with external “integrat.exe” engine for level IV simulations. Also, the EU TGD EUSES spreadsheet has a model tab for level IV simulations.

Option 2

- The Unit World Model (UWM) tool has the additional metal fate processes included in the freshwater and sediment compartment programmed in a stand-alone software (Farley et al., 2011). The UWM is using information from MINEQL+ and WHAM software.
- The IDMM (Intermediate Complexity Model for Metals) is a model for long term metal dynamics in the soil compartment (Lofts et al., 2013).

22.6. Priority level

1. Number (type of) of chemicals affected: Number (type of) of chemicals affected: low (metals/inorganics) but high tonnage chemicals with high need under REACH Authorization process
   Substances affected
   Option 1: Chemicals for which steady-state concentrations are reached at a long time scale: metals/inorganics but could be broader. (e.g. persistent)
   Option 2: Inorganic compounds (metals)
2. Maturity: Scientifically documented: yes for option 1 and 2
3. Implemented into IT tool : yes for option 1 and 2

4. Regulatory considerations: option 1: expected increasing need under REACH Authorization process to regulate specific uses (under REACH registration of metals, measured data covering all uses are typically used to estimate PECregional hereby), option 2 needs Guidance update
5. Expected impact on exposure: be able to calculate more realistic PECregional for metals
6. New data requirement: no for option 1, yes for option 2

Suggested priority:

- Option 1: Ready/ High importance for metals
- Option 2: Not ready/ High importance for metals

22.7. References

Farley KJ, Carbonaro RF, Fanelli CJ, Costanzo R, Rader K, Di Toro (2011) TICKET-UWM: a coupled kinetic, equilibrium, and transport screening model for metals in lakes. Environmental Toxicology and Chemistry 30(6), 1278-1287.

Lofts S, Tipping E, Lawlor AJ, Shotbolt L (2013) An intermediate complexity dynamic model for predicting accumulation of atmospherically deposited metals (Ni, Cu, Zn, Cd, Pb) in catchment soils: 1400 to present. Environmental Pollution 180, 236-245.

23. Bioavailability of metals

23.1. Current situation in EUSES

The current EUSES model allows only to distinguish the total dissolved and particulate fractions of the substances. Although this approach is appropriate for the neutral organic compounds it typically overestimates the actual bioavailability and toxicity of metals and thus does not support metals risk assessment in an appropriate way.

To correct this erroneous routine for metals, current risk assessment practice under REACH and BPR uses different bio-availability "correction" factors (ECHA Guidance R.7.13-2). Most of them are currently considered at the effect assessment (PNECs). In addition, for sediment and soil compartment, some bio-availability correction factors are applied in the exposure assessment (e.g. Acid Volatile Sulfides (AVS) binding in sediment and ageing factor in soil). Despite all above such corrections are still applied just a posteriori, in addition they might be done only outside EUSES.

Some environmental impact models (e.g. USEtox) have already started to include speciation modelling in the environmental fate model to estimate the "truly dissolved" form. This approach considers only the part of the total dissolved metal concentration (free ions species and inorganic complexes) and excludes the colloidal (DOC-bound) form (Fig. 1) (OECD 2016; Diamond et al. 2010; ICMM 2016). This speciation modelling takes also into account the site-specific chemical conditions (pH, DOC, major cations and anions, etc. of environmental compartment), which is not possible in EUSES.

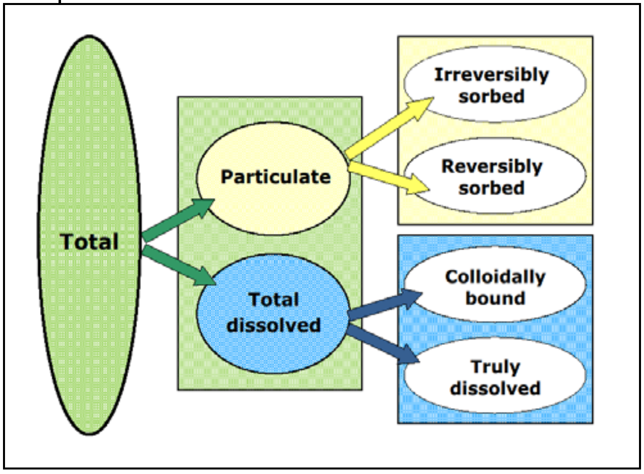


Figure 11: Fractions of metals

23.2. Change proposed (why and what)

The "bioavailability" concept encompasses several operationally defined and interacting processes (see Fig. 2). Availability starts with physico-chemical considerations (environmental availability – speciation modelling) but should be subsequently linked to different ecological receptors taking different uptake routes into account (ECHA, 2014; OECD, 2016). Since the correction of metals bioavailability should be done for both the exposure and effect side (OECD 2016; ECHA Guidance R.7.13-2), the following considerations are proposed for the further discussion.

Exposure:

In contrast to the neutral organic substances, for which solids-water partition coefficients may be calculated in EUSES (based on the log Kow), Kp values for metals could be derived using appropriate geochemical models (e.g. WHAM). Consequently, EUSES could not have to be supported by measured data. Given the spatial variability in the EU (freshwater, sediment and soil compartments of different physico-chemical combinations), the calculations need to be conducted for several physchem combinations, i.e. so-called biogeochemical regions (OECD, 2016) or eco-regions (EU RAR).

Effect:

To reflect actual metals toxicity and to compare both PEC and PNEC within bioavailability concepts it is proposed to use the BLM models (Figure 12).

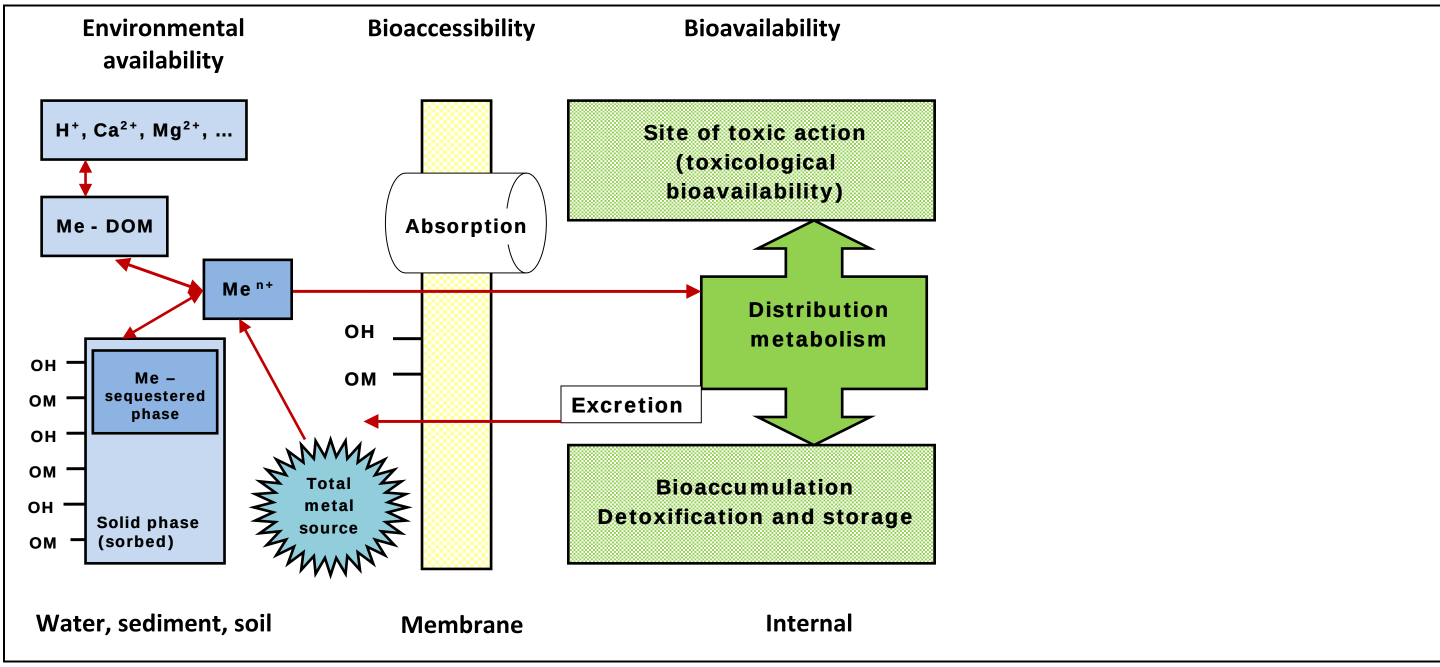


Figure 12: Simplified conceptual outline for metals bioavailability

Why needed?

The degree to which metals are available and cause toxicity to aquatic, sediment-burying and terrestrial organisms is determined by site-specific geochemical conditions controlling the speciation/precipitation and/or complexation of metals. In the aquatic environment, these processes are generally controlled by pH and DOC (dissolved organic carbon). Furthermore, several cations (Ca, Mg, Na, K) are known to compete with metal ions for binding to the site of toxic action and have the potential to reduce metal toxicity. In sediments, sulfides, organic carbon and iron/manganese (oxy)hydroxides play a mitigating role as they provide important binding/absorption phases. For the soil compartment, it has been demonstrated that clay minerals, organic carbon and soil pH are the main drivers controlling bioavailability of metals. The wide variation of the physico-chemical characteristics encountered in the environment is the main reason why no clear relationships have been observed between measured total concentrations of metals and their potential to cause toxic effects. Therefore, taking bioavailability into account will improve traditional environmental assessment approaches as it helps to increase the realism of the assessment and can help regulators to better understand the likelihood of the occurrence of adverse effects due to metal contamination.

23.3. Support for implementation

- ECHA. 2008. Guidance on information requirements and chemical safety assessment. Appendix R.7.13-2: Environmental risk assessment for metals and metal compounds. July 2008.
- ECHA. 2014. Principles for environmental risk assessment of the sediment compartment. Proceedings of the topical scientific workshop. Editors: Tarazona JV, Versonnen B, Janssen C, De Laender F, Vangheluwe M and Knight D. Associated Editors: Ape D, Burgess RM, Carere M, De Knecht J, Ddier L, Gwalik B, Karjalaine AM, Kukkone J, Peijnenburg W, Pellizati F, Salvito D, Schlekat C, Sibly P, Simpson SL, Tyle H, Waeterschoot H and Weltje L. ECHA-14-R-13-EN.
- Gandhi N, Diamond M.L., Van de Meent D., Hujibregts, M., Pejinenburg W., Guinee J. (2010): New method for calculating comparative toxicity potential of cationic metals in freshwater: application to copper, nickel and zinc. Environmental Science and Technology. Vol. 44, No. 13.2010.

- Diamond et al. (2010): The clearer consensus: the estimation of metal hazard in fresh water. Int. J. Life Cycle Assess 15(2):143–147.
- ICMM. (2016). Metals Environmental Risk Assessment Guidance. Fact sheet 5: bio-availability: water, soil and sediment. (https://www.icmm.com/merag)
- OECD (2016). Guidance on the Incorporation of Bioavailability Concepts for Assessing the Chemical Ecological Risk and/or Environmental Threshold Values of Metals and Inorganic Metal Compounds. OECD Series on Testing and Assessment No 259. ENV/JM/MONO(2016)66.
- USEtox® 2.0 Documentation (http://www.usetox.org/sites/default/files/assets/USEtox_Documentation.pdf)
- BPR Guidance Vol. IV part B+C chapter 4.5.1. (in general aspects)

23.4. Priority level

1. Number (type of) chemicals affected: low (metals) but with high tonnage;
2. Maturity of the improvement: presented approach is scientifically documented for some metal species (Cu, Zn, Ni especially) but must be further investigated for the other metals;
3. Implementation in IT tools: USEtox model (only speciation modelling);
4. Regulatory considerations: current regulatory guidances refer only to the general aspects on the metals bioavailability (OECD, ECHA); further validation and detailed discussion
   on the presented implementation approach has to be considered at the regulatory level (e.g. on the physico-chemistry scenarios to be considered);
5. Expected impact on exposure: better, more realistic estimation of the PEC (and PNEC) values for metals;
6. New data requirement: yes, scientific research on the metal bio-availability needs

Suggested priority: Not ready/ highly importance for metals

Bioavailability concept of metals based on the truly dissolved fraction within specific geochemical conditions has been extensively documented in the numerous scientific studies (for Cu, Ni and Zn especially), and so far it has partly been implemented into USEtox model and used by means of *a posteriori* correction factors in current risk assessment practice. For the above reason it is proposed to initiate a discussion for such adaptation in EUSES . The complexity of this issue requires however several regulatory agreements as a first step. The main (and possibly not the only) questionsunder consideration should be thus the following:

- choice of the average /worst-case biochemical regions for each kind of metal/ in the UE (representative pH, DOC, alkalinity, etc. of the environmental compartments; number of representative regions);
- validation and agreement on the choice of geochemical speciation (e.g. WHAM) and BLM models;
- method of EUSES update (Kp and PNEC values derivation outside EUSES or implementation of the agreed tools into EUSES).

It is also suggested that refined risk assessment for metals based on their true bioavailability should be done in parallel with the metal-specific fate processes (as presented in the topic 21).

24. Consideration of natural background concentration for inorganics

24.1. Current situation in EUSES

The current version of EUSES does not explicitly consider the natural background concentration for natural occurring substances like inorganics despite it needs to be taken into account. According to the ECHA Guidance Appendix R.7.13-2 and the technical agreements taken during the approval stage of the biocidal active substances of natural origin, in such cases Added Risk Approach (Added RA) or Total Risk Approach (Total RA) has to be considered. In the Added RA only the anthropogenic (e.g. biocidal) exposure is taken into account. Then PEC is compared to the PNEC and to the natural background concentration. In case of the Total RA – release due to anthropogenic use is added to the background (natural-pristine and/or regional) concentration and then these “total” PEC is compared to adequately derived PNEC.

24.2. Change proposed (what and why)

To avoid manual calculations in the Total Risk Approach with the background concentrations outside EUSES (mainly under BPR) it is proposed to explicitly implement natural and/or regional background concentrations into EUSES as follows:

$\text{PEClocal}_{\text{compartment, total}} = \text{PEClocal}_{\text{compartment, added}} + \text{PECregional}_{\text{compartment}} + \text{PEC natural/pristine}_{\text{compartment}}$[17]

24.3. Support for implementation

Reference can be made to existing metal chemical safety/risk assessment under REACH and inorganic active substances of natural origin under the BPR (already evaluated by EU Member States).

ECHA Guidance Appendix R.7.13-2: environmental risk assessment for metals and metal compounds (https://echa.europa.eu/documents/10162/13632/information_requirements_r7_13_2_en.pdf)

24.4. Priority level

Criteria for priority evaluation:

1. Number (type of) of chemicals affected: natural occurring substances (metals and other substances of natural origin): low number but very high tonnage under REACH and many product authorisations under the BPR

1. Maturity: Scientifically documented: yes
2. Implemented into IT tool: not relevant due to simplicity of equations
3. Regulatory considerations: not needed; presented approaches are already agreed under REACH and BPR
4. Expected impact on exposure: none since in the majority of cases natural regional concentrations considered through workarounds.
5. New data requirement: no

Suggested priority: Ready/high importance for natural substances

To reflect appropriate $\text{PEC}_{\text{compartment}}$ values for inorganic substances of natural origin background concentration must be taken into account. Such possibility is currently not available in EUSES although it is required under REACH and BPR. Since the presented approach is simple for implementation, agreed (at both scientific and regulatory level) and needed for many biocidal products and substances with a high tonnage the proposed update in EUSES is ready for the implementation with a high priority score.

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[17] In cases where only natural –pristine concentration should be added to $\text{PEClocal}_{\text{compartment, added}}$ cells relevant for $\text{PECregional}_{\text{compartment}}$ will have to be set by 0 value. The same would apply in cases where only $\text{PECregional}_{\text{compartment}}$ must be added to the $\text{PEClocal}_{\text{compartment, added}}$.

25. Parallel assessment (for multi-constituent substances and for substances transforming on use/ in STP)

25.1. Current situation in EUSES

The current version of EUSES contains the so-called Hydrocarbon Block Method (HBM) module which enables the parallel exposure and hazard assessments of defined “blocks”. This module had been developed to support the assessment of multi-constituent chemicals (initially hydrocarbons). The following steps had been defined for the assessment:

- Blocks can be defined by grouping constituents on the basis of structural similarity and similar physico-chemical/ecotoxicological properties (blocks can be defined as single constituents also). Representative values for physico-chemical properties, degradation-rate constants and LC/EC50s/NOECs are assigned to each block (or to each constituent).
- Release estimation for each block is performed by the tool on the basis of the information on the tonnage of the substance and fraction of the block present in the substance.
- Then PECs and PNECs for each protection target are estimated for each block. PEC/PNEC ratios for each block are summed up per protection target to estimate a risk characterisation ratio of the multi-constituent chemical.

25.2. Change proposed (why and what)

Parallel assessment is a concept, which can be applied to a number of other cases apart from hydrocarbons, for example:

- assessment of multi-constituents chemicals (or UVCBs where several “blocks” may be defined)
- assessment of several substances being part of a mixture
- assessment of substance and its transformation product[18]

Multi-constituent and UVCB substances make a big share of the REACH substances. E.g. based on the information reported in IUCLID ~ 25% of registrations are for UVCB substances. Multi constituent and UVCB substances are also numerous in biocides. In addition the assessment of biocidal products must consider the whole mixture, i.e. all active substances and substance(s) of concern. Thus, to ensure functioning of REACH and BPR hazard/exposure/risk assessment approaches need to be available for multi-constituent chemicals and mixtures.

No conceptual changes are proposed for the assessment of multi-constituent substance as comparing to the already available HBM module, which could be used for a wider spectrum of multi-constituent chemicals and not only hydrocarbons (when necessary assessment could be based on the consumption rates and not tonnage information).

Furthermore the assessment of transformation and degradation products is part of REACH and BPR requirements (see REACH Annex I, section 5.2.4. and BPR Annex VI[19]). Also for BPR, in case of active substances generated *in situ* the active and its precursor(s) shall be assessed in parallel.

To note that for REACH purposes the Chesar tool has implemented a risk assessment approach, based on the so-called assessment entities[20], for the multi-constituent/UVCB substances and transformation products which follows the logic and principles of the HMB module. In Chesar such assessment is enabled by introducing separate properties data sets (via assessment

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[18] Parallel exposure assessment of parent substance and transformation product(s) can be carried out using HBM. A worst case assessment could be done by assessing 100% of parent and 100% of transformation products (then the PEC/PNEC ratios should not be summed up but looked in parallel). Alternatively a specific percentage of parent and transformation product(s) may be set [if parent degrades in the STP 100% for the parent and the percentage of transformation product(s) assumed to be formed].

[19] See also the guidance for biocides Vol. IV part B+C

[20] The assessment entity in IUCLID is a wrapper [container] for a set of substance property data used for assessment purpose across all endpoints. It enables the assessor to define consistent datasets of properties that are relevant for specific compositions/forms (placed on the market or generated upon use). These datasets are then used to assess the substance over its life cycle, considering its chemical behaviour in the different foreseen uses.

entities). Those data sets can correspond to the properties of various constituents of a substance or to the properties of the transformation product(s) and/or parent substance. The proportion for each of those elements (based on the composition of the substance or its transformation rate) should be set by the assessor.

The HBM module in EUSES could be used in a same way for assessing parent substances and transformation products (static parallel assessment only possible where no temporal variations taken into account). Therefore we suggest that the HBM module:

- unlocked for biocides and adapted for their ESDs
- renamed more generically to reflect its usability for UVCB substances, mixtures, etc. falling under REACH and biocides Regulations.

25.3. Support for implementation

As mentioned above the concept of parallel exposure assessment for a number of constituents/substances (called blocks, assessment entities) is implemented in EUSES HBM module and in Chesar.

Further information is available for multi-constituent chemicals:

- See documentation available for download and, more specifically, Chapter III, section 8 on Hydrocarbon Block Method: https://ec.europa.eu/jrc/en/scientific-tool/european-union-system-evaluation-substances
- Chesar manual (see chapter 9): https://activity.echa.europa.eu/sites/act-6/process-6-4/06.04.04/docs/02_ChesarToolDevelopment/03_Chesar3/05_ReleasePackage/03_UserManual/Chesar3.3 UM/Chesar33_user_manual.doc
- IUCLID manual for registration (see section on assessment entities): https://echa.europa.eu/documents/10162/22308542/manual_regis_and_ppord_en.pdf/891754cb-a6b6-4bb6-8538-52ccde74070e
- PETRORISK spreadsheet tool: http://www.concawe.eu/reach/petrorisk/

25.4. Priority level

1. Number (type of) of chemicals affected: multi-constituent and UVCB substances under REACH and BPR where more than one (block of) constituent is of concern; biocidal product containing more than one active substance and substance(s) of concern; substances transforming during use or in the STP (including substances generated in situ and their precursors);
2. Maturity of the improvement: the principal approach is already developed and accepted within REACH and BPR in EU and by some other jurisdictions (e.g. Canada).
3. Implementation in IT tools: Implemented in the EUSES and in several other tools Chesar and PETRORISK (together with further adaptations which are documented- see in section 24.3).
4. Regulatory considerations: The principles of risk assessment for multi-constituent substances are agreed and accepted under REACH and BPR (a number of indications are available in relevant pieces of Guidance documents).
5. Expected impact on exposure and/or alternative solutions available: No impact on exposure for REACH substances since the scenario has been already implemented in EUSES. However, the proposed change would facilitate exposure assessment for the biocides uses.
6. New data requirement: Set of data necessary for each constituent of multi-constituent chemical/each transformation product to be assessed (in addition, proportion of the different “block” is needed).

Suggested priority: Ready/high importance

The possibility for parallel exposure/risk assessment is currently available via the HBM module in EUSES, but has to be made available for biocides assessment. As the assessment of multi-constituent and UVCB substances for REACH and BPR, of mixtures of several active substances/substances of concern in biocidal products, as well as assessment of parent substance and transformation products (or substances generated in situ with precursors) are legally required, further development of this assessment module in EUSES is of high priority and ready for the implementation.

26. Assessment of substance transforming in the environment

26.1. Current situation in EUSES and why should the topic be explored

The assessment of transformation and degradation products is part of REACH and BPR requirements (see REACH Annex I, section 5.2.4. and BPR Annex VI[21]). Also for BPR, in case of active substances generated *in situ* the active and its precursor(s) shall be assessed in parallel. However, there is no module currently available in EUSES which would enable exposure/risk assessment for the transformation products and/or parent substance when degradation/transformation in the environment (taking account of non-equilibrium concentrations of these chemicals). Therefore such scenarios should be further developed and implemented in the tool (longer-term perspective).

As noted in the RIVM report[22] various studies have pointed out how parent-transformation products relations can be modelled in environmental fate and how existing models can be adapted to include prediction of exposure concentrations for transformation products of the parent compound (Fenner et al., 2002; Cahill et al., 2003; Van Zelm et al., 2010; Franco et al., 2011; Ng et al. 2011). An example is the study by Van Zelm et al. (2008), who have created a multi-species version of the EU TGD spreadsheet to serve industry in analysing the environmental fate of perfluorinated octanoic acid (PFOA) based chemical substances. However, it should be noted that modelling of exposure of transformation products occurring in the environment would mainly have an impact on the regional exposure concentrations. There is no impact on predicted local concentrations in waters and sediments estimated by the current release scenario for REACH. Only local concentration in soil would be affected following the application of sludge from STP. However, such modelling of transformation products in soil might be of interest for only stable and toxic transformation products.

26.2. What is proposed

Our proposal is to explore the need for refining the assessment methods when substances are transformed in the environment for REACH substances and biocides.

Further information is available for assessment of parent substance and transformation products:

Van Zelm et al. (2008) have implemented multi-species mass balance modelling in the EU TGD spreadsheet, which closely follows EUSES 2.0. A similar implementation was done in the OSIRIS project, documented by Ng et al. (2011), however using a different format.

26.3. Priority level

1. Number (type of) of chemicals affected: limited number of substances by-passing STP which would undergo transformation in environmental compartments and could not be assessed using the parallel assessment approach. During development of the approach it still needs to be clarified when such assessment would be triggered – e.g. substances by passing STP and transforming into persistent and/or toxic products in the environment.
2. Maturity of the improvement: There are initial guiding principles and methods available, however not further validated.
3. Implementation in IT tools: unclear at this stage.
4. Regulatory considerations: Bearing in mind that the modelling of exposure of transformation products occurring in the environment would mainly have an impact on the regional exposure concentrations, the regulatory relevance of the assessment of transformation products formed in the environment still needs to be agreed. If relevant, methodology needs to be further discussed and accepted for the regulatory use.

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[21] See also the guidance for biocides Vol. IV part B+C

[22] Dik van de Meent et al., Identification an preliminary analysis of update needs for EUSES. National Institute of Public Health and the Environment (RIVM), Netherlands under Contract No ECHA/2014/253.

5. Expected impact on exposure and/or alternative solutions available: Once accepted and implemented, exposure/risk assessment would be enabled for a transformation products of concern (e.g. persistent and toxic) for a number of substances which would undergo transformation in the environment.
6. New data requirement: Set of data for the parent substance and each transformation product of concern.

Suggested priority: Not ready

With regard to simultaneous exposure assessment of parent substance and environmental transformation products, there is a need for further validation of available principles and methodology of such modelling as well as regulatory relevance and acceptance of it needs to be further discussed and endorsed. Furthermore, it should be noted that this update would affect a limited number of the substances transforming in the environment into products of concern. Therefore, this update would merit medium priority with implementation in a longer-term perspective.

26.4. References

Cahill TM, Cousins I, Mackay, D (2003) General fugacity-based model to predict the environmental fate of multiple chemical species. Environ. Sci.Technol. 22(3)483-493.

Franco A et al., (2011) OSIRIS Deliverable D3.1.17 (6th Framework Program, EU, Project no. 037017) Recommendations for adaptations of ECHA Guidance Documents and EUSES.

Fenner K, Cornelis Kooijman, Martin Scheringer, Konrad Hungerbühler. (2002). Including Transformation Products into the Risk Assessment for Chemicals: The Case of Nonylphenol Ethoxylate Usage in Switzerland. Environ. Sci. Technol. 36, 1147-1154.

Ng et al. (2011). OSIRIS Deliverable D3.1.15 (6th Framework Program, EU, Project no. 037017) Comparison of new models for multispecies compounds (including ionisable compounds and degradation products) to existing ones.

Van Zelm R, MAJ Huijbregts, D van de Meent. Transformation products in the life cycle impact assessment of chemicals. Environmental Science and Technology, 44(2010), 1004–1009. (link to the publication: here)

Van Zelm R, MAJ Huijbregts, MH Russell, T Jager, D van de Meent. 2008. Modeling the environmental fate of perfluorooctanoate and its precursors from global fluorotelomer acrylate polymer use. Environmental Toxicology and Chemistry, 27(2008), 2216-2223. (link to the publication: here)

27. Aggregate local exposure assessment (biocides)

27.1. Current situation in EUSES

Article 19(2) of the new Biocidal Products Regulation (BPR, 528/2012 EU) states that “the evaluation […] shall take into account the following factors: […] (d) cumulative effects, (e) synergistic effects.” This is further elaborated in Annex VI (common principles for the evaluation of biocidal products) which states that the risks associated with the relevant individual components of the biocidal product shall be assessed, taking into account any cumulative and synergistic effects.

There is currently no agreed guidance in place and no possibility to perform an assessment of cumulative effects (including quantitative aggregated local exposure assessment by summing up of PEC/PNEC values for one substance from several uses) for biocides.

A draft guidance document on aggregated exposure assessment is currently under discussion by the BPC Environment Working Group and estimated to be finalised by end of 2018.

Currently exposure assessments are done for biocides in EUSES for single uses and the aggregated exposure assessment is performed outside EUSES.

27.2. Change proposed (why and what)

We propose to have the possibility to assess several uses for the same active substance in one assessment (within one PT as well as between different PTs) and to indicate (e.g. tick box) during the assessment of individual uses whether the outcome is relevant for aggregated exposure assessment, i.e. the marked PEC/PNEC values are then summed up for a given protection target. Note that such aggregation should only be made when there is overlap of exposure in time and space. Therefore only exposure in same receiving compartments can be summed up.

Within the process of evaluation of dossiers for biocidal products, as specified in Annex VI of the BPR, the possibility of aggregated exposure must be taken into account (BPR Article 8(3) and Article 19, 2(c)) (see section 4.4).

An aggregate exposure assessment should be conducted for a biocidal active substances when there is exposure:

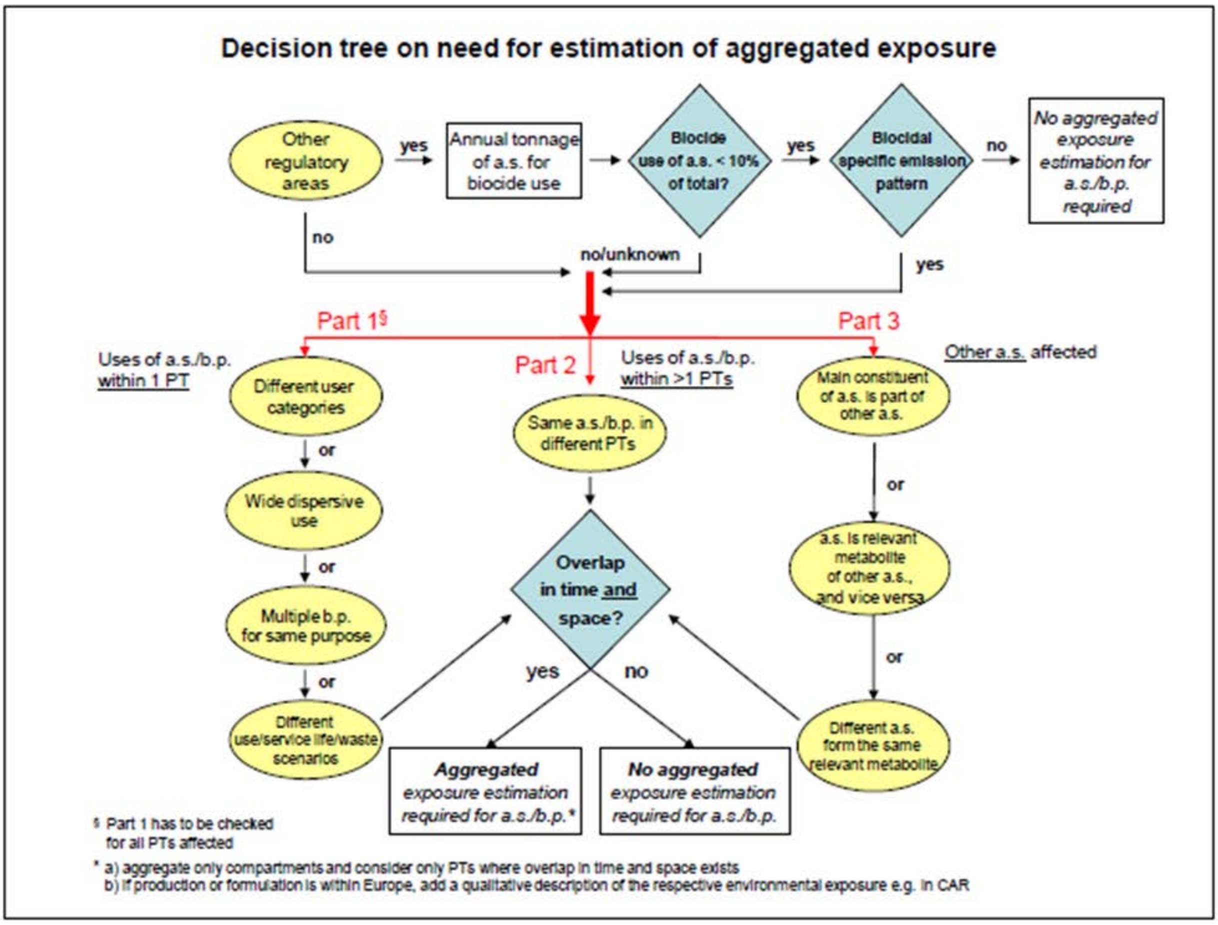
- through more than one release pathway,
- through more than one use (e.g. professional and non-professional),
- that is used in more than one PT

Note that in Chesar supports the local assessment of the sum of all widespread uses. The simultaneous use at a given site in nevertheless is not yet supported in the current version of Chesar.

27.3. Support for implementation

- Publications *:*
  - o ECHA Guidance on Biocidal Products Regulation: Volume IV Environment - Assessment and Evaluation (Parts B+C) (version 2.0 October 2017).
  - o Hermann, A., and Merwede. J-H. (2016). Aggregated Environmental Exposure Assessment and Risk Characterisation of Biocidal Products – Legal Aspects. German Federal Environment Agency. Project No. (FKZ) 3711 63 412.

- Specific guidance for performing an aggregated exposure assessment is currently under preparation, the finalisation is preliminary scheduled for Q4 2018. So far, the following decision scheme has been discussed and agreed to assess the need for conducting an aggregated exposure assessment:



Decision tree on need for estimation of aggregated exposure

§ Part 1 has to be checked for all PTs affected

* a) aggregate only compartments and consider only PTs where overlap in time and space exists
b) if production or formulation is within Europe, add a qualitative description of the respective environmental exposure e.g. in CAR

Figure 13:Decision tree for aggregated exposure assessment for biocides (Competent Authority Report (CAR) template)

27.4. Priority level

1. Number (type of) of chemicals affected: Mainly biocidal active substances and their metabolites as well as pre-cursors or substances of concern in biocidal products are concerned.
2. Exposure impact at local scale for biocides.
3. Maturity of the improvement: Guidance on aggregated exposure assessment is under preparation, currently documented in a decision tree (see Figure 1).
4. Implemented into IT tool: Not yet implemented in IT for biocides. A similar concept is implemented for REACh in Chesar for some situations.
5. Regulatory considerations: No impact for biocides (already mentioned biocides guidance under preparation).
6. New data requirement: No new data required.

Suggested priority:

Nearly ready /High importance for biocides according to ECHA since the proposed change fills a gap and introduces concept of aggregated exposure assessment on local scale in EUSES.

Reservations from ECETOC.