

“EUSES update” workshop (4-5 June 2018)

1. Introduction

1.1. Background

EUSES (the European Union System for the Evaluation of Substances) enables government authorities, research institutes and Industry to carry out assessments of the risks posed by chemical substances to the environment and man via the environment. It is used for almost all the environmental assessments under REACH and for all the assessments for biocides. EUSES is an assessment methodology as well as a tool. Under REACH the principles of environmental exposure assessment, largely aligned with EUSES, are described in the Guidance on information requirements and Chemical Safety Assessment; Chapter R.16: Environmental exposure assessment¹. The situation is similar for biocides, where the principles are reported in the guidance on the Biocidal Products Regulation, Volume IV Environment-Assessment and Evaluation (Parts B + C)². The relevant elements of the EUSES methodology are embedded in the most used REACH tools (Chesar and EasyTRA) and for Biocides the full EUSES tool is used as such.

EUSES was originally developed by the authorities³ in the 90's to support environmental exposure assessment for new chemicals, existing chemicals and biocidal active substances in line with the methods described in the Technical Guidance Document (TGD) that harmonised the assessment practices for these three policy areas. The availability of such a single harmonised tool significantly improved the consistency of the assessments both within and between these policy areas. The increased consistency also had a positive impact on the quality and transparency of the assessments as well as on the efficiency of preparing them. This in turn increased the efficiency of evaluating the assessments. However, EUSES has not been actively maintained recently, so no further development has been carried out since 2012. This has led to the situation that the tool is starting to get outdated both methodologically and technologically. Furthermore, note that some divergence between biocides and REACH has occurred in the last years and it would be beneficial to keep as much consistency as possible between those two areas.

At the moment, ownership of EUSES lies with the DG JRC. ECHA has decided to take over the ownership of the tool. In order to take further decisions on how to proceed, ECHA has to assess the consequences in terms of resources and budget of further developing and maintaining it. Note that ECHA is now implementing a “quick fix” in the current version of EUSES in order to better support the biocides needs. Specifically, this includes the implementation of a number of Emission Scenario Documents and will be available by end of 2018.

1.2. EUSES development plans

Apart from the “quick fix”, ECHA has not taken commitment yet with regard to EUSES update and maintenance, therefore the plans described here will have to be confirmed after the Workshop.

The ultimate objective is to update and maintain EUSES to adequately support environmental

¹https://echa.europa.eu/documents/10162/13632/information_requirements_r16_en.pdf

²https://echa.europa.eu/documents/10162/23036412/bpr_guidance_ra_vol_iv_part_b-c_en.pdf/e2622aea-0b93-493f-85a3-f9cb42be16ae

³ Originally the predecessor of the EUSES tool was developed by RIVM in the Netherlands. This development was taken over by the European Commission (JRC).

assessors, bringing consistency between REACH and biocides regulations (and possibly beyond those 2 regulations). For that, the EUSES tool would have to be redeveloped in order to facilitate its maintenance and update in a new IT technology. In a first step the concepts, algorithms and functionalities available in the tool would not be changed. However while implementing REACH and the Biocides Regulation over the last years, the need for some modifications in the current tool has been identified. A number of changes have been identified by the organising committee for the workshop⁴ and will be presented and discussed at the workshop. They are listed in section 5 and further described in annex 2 to this document. In parallel to the potential implementation of such first set of modifications, a process for collecting and assessing additional needs for improvement in a longer term perspective will have to be set in place. This process should ensure that the various stakeholders are properly involved.

The following first steps are foreseen, so that ECHA can take a decision on whether, to which extent, and how it should take the responsibility of updating and maintaining EUSES:

- A workshop with stakeholders (4-5 June 2018) to present and collect ideas on needs to update EUSES. It will also be an opportunity to collect feedback on a proposal describing how the various stakeholders could be involved in the process of updating EUSES (in particular industry and authorities dealing with regulatory environmental exposure assessment within REACH and biocides but also academia and other interested parties)
- An pre-study launched by ECHA to analyse the needs and propose solutions with a related cost estimation for the update of EUSES [possibly in Q4 2018- Q2 2019]. Such study will include:
 - An analysis of what would be the best way to develop and deliver EUSES within the landscape of other tools it should interact with, in particular Chesar (see section 3).
 - An analysis and design of the requirements for the first version of the tool. Such first version is expected to largely enable the functionalities and calculations supported by the current version of EUSES, modified and adapted on the basis of new requirements presented and discussed at the workshop.
- A decision will then be taken by ECHA on whether to redevelop a first version of EUSES in modern IT technology
- If such redevelopment is done [possibly between Q4 2019- Q3 2021] then further development and maintenance of EUSES will have to be considered.

It is important to ensure that the various stakeholders are involved and can contribute along the full process.

2. Purpose of the workshop

The primary objective of this workshop is to review the state of the art regarding environmental exposure assessment of chemical substances in view of a EUSES update to better support regulatory assessment under REACH and Biocide Product Regulation. The workshop will provide a platform for regulators, industry, academia and other stakeholders of REACH and Biocides Regulations to address the needs for an update of EUSES and on the means to do so. The discussions will be based on the recent scientific developments in release estimation and fate assessment within regulatory exposure assessments.

The specific objectives of the workshop are:

⁴The organising group for the workshop consists of Industry representatives: Frederik Verdonck (Arche Consulting) for Eurometaux, Paul Mason (Sc Johnson) for Cefic, Erwin Annys (Cefic), Johannes Tolls (Henkel) then replaced by Diederik Schowanek (Procter and Gamble) for ECETOC, member states representative: Joost Bakker (RIVM, NL) Anna Hadam (PL MSCA; biocides), Sara Martin (UK. Only joining very lately) and ECHA representatives: Hélène Magaud, Romanas Cesnaitis, Stefano Frattini, Eleni Tsitsiou, Heike Schimmelpfenning and Eugenia Nogueiro

- Discuss and agree among stakeholders from industrial chemicals and biocides areas on some initial update needs (for both release and fate modelling modules) for EUSES from a content perspective, with a view for IT implementation. A list of topics is proposed by the organising committee of the workshop and the relevance of those topics as well as the priority of those will be discussed at the workshop. The priority should take into account the relevance of the update, easiness of implementation and agreement on the solution among stakeholders (see section 5).
- Collect additional ideas on needs for updates from the participants of the workshop
- Discuss a proposal for the stakeholders' involvement during the update and maintenance of EUSES by ECHA. This proposal should cover the stakeholders' involvement for defining requirements (and their priority), providing input when relevant to the IT-developers, testing the tool and providing the adequate guidance for the tool (see Annex 1).

3. IT development aspects and relationship to Chesar

In order to best support users of EUSES in the future an analysis of how is EUSES used and how it is expected to be used in the future will have to be carried out.

As explained above, options to re-develop EUSES will be analysed in a pre-study to be launched in Q4 2018. Nevertheless the following considerations are to be taken into account for the pre-study:

- It may be preferable that functionalities available in other tools (e.g. IUCLID, Chesar, QSAR tools) are not redeveloped in EUSES. The interaction between EUSES and those tools should be considered.
- In particular a number of functionalities which may be relevant for EUSES (e.g. connection with IUCLID, SPERCs, documenting choices and approach, advanced reporting functionalities, see below) have been implemented in Chesar

Chesar is a tool developed and maintained by ECHA to support registrants under REACH to carry out their chemical safety assessment, generate their Chemical Safety Report (CSR) and related Exposure Scenarios to be annexed to the Safety Data Sheet. It is now used for generating more than 50% of the CSRs. The key steps implemented in Chesar are:

- Importing the relevant substance properties from IUCLID
- Enabling the description of the uses of a substance for its full life cycle. For each use, corresponding to a given life cycle stage, a number of contributing activities are described from the environment and workers and/or consumers perspective.
- Carrying out exposure assessment for each contributing activity for the environment (exposure assessment for workers/consumers is also covered but not described in this document):
 - default estimates for the releases are provided on the basis of total use tonnage and Environmental Release Categories (ERCs) but refined estimates for the releases can also be used. A description of the conditions of use related to such release has to be provided in order to generate an exposure scenario
 - exposure is then estimated for the various target compartments making use of the fate and distribution calculation engine of EUSES
- Generating CSR and ES for communication.

Note that Chesar supports some initial tiering of the exposure assessment in a transparent way:

- Whether man *via* the environment is to be assessed is set up in Chesar *via* a manual justification based on the criteria provided in the REACH IR&CSA guidance, chapter R.16

- The release estimation method is to be specified: the releases are based on ERCs by default, but releases can also be based on SPERCs⁵ or on manually provided release factors or release rates. The “site” tonnage is calculated by default (from use tonnage or SPERC information) but can be manually overwritten. Explanations can be provided systematically when some defaults are changed and are reported for transparency in the CSR.
- A few parameters such as the selection of the receiving environment (freshwater or sea), the dilution into the receiving environment, the biological sewage treatment plant (STP) settings (see below) can be modified, but only for “site specific uses”⁶ (for site-specific assessment)
- Release fractions from the biological STP are by default calculated by EUSES (based on SimpleTreat 3.1), but can also be manually entered when substance specific data, valid for any site or for a specific site, exists (e.g. from results of simulation test)
- The biological STP settings (flow rate, application of sludge on soil) cannot be modified except for “site specific uses”.
- Other EUSES default parameters cannot be modified in the current version of Chesar

In addition, it should be noted that **IUCLID** serves as a database in particular to record the properties of substances. A number of those properties are used as input to EUSES: physico chemical and fate properties but also PNECs (a PNEC calculator is also included in IUCLID). Those data can be imported directly into Chesar. If needed, a direct import of those data from IUCLID to EUSES could be envisaged as an option (see section 4.1) when EUSES is not used in combination with Chesar. Figure 1 illustrates the exchange of data between the various applications.

⁵ SPERCs are Specific Environmental Release Categories, providing release factors that can be assumed for a specific use under a defined set of conditions for that use. They are developed by sector associations.

⁶ For widespread uses such as uses by consumers such settings cannot be modified by the assessors within Chesar.

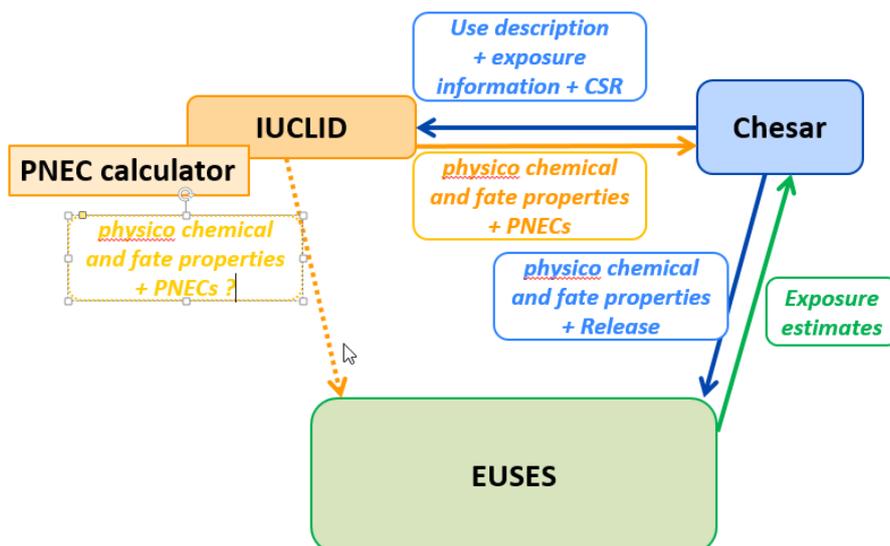


Figure 1: Exchange of data between the various tools

4. Overview of EUSES modules

4.1. High level description of various EUSES modules

In the context of this work only the modules related to the assessment of environment and man via the environment are considered⁷.

Figure 2 describes at a very high level the structure of the tool.

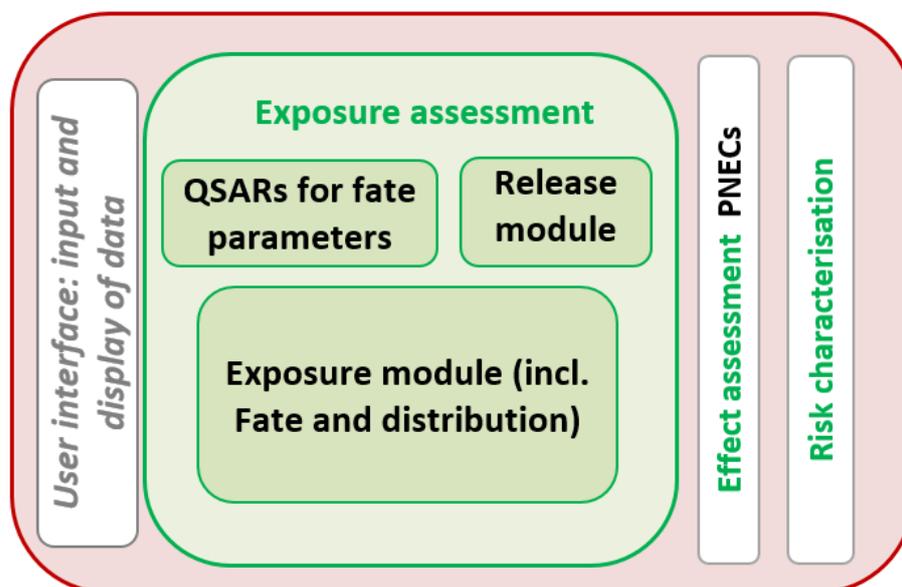


Figure 2: High-level description of the structure of EUSES

EUSES is composed of several modules (note that when redeveloping the tool some modifications may be introduced to what is described below):

- **Exposure assessment:** Based on information on the properties of the substance, and the release rates (amount per time) per route, exposure estimates are derived for various compartments.

⁷ In the current EUSES also an old version of Consexpo and EASE are included. Consexpo now exists in a newer version and EASE is not maintained. Therefore those two software will not be considered.

- As a minimum the molecular weight, water solubility, vapour pressure, octanol/water partition coefficient (Kow) (or adsorption-desorption coefficient (Koc) and measured BCF value) and the results of screening tests on biodegradability are currently needed. The current EUSES version integrates **QSARs** to estimate Koc and BCF based on Kow, if no specific data are available.
- The **release module** covers the estimation of the amount directly released via different **release routes (release rate)** into a **receiving compartment** such as waste water, freshwater/marine water, air, industrial or agricultural soil.
- Release rates are used as input parameters to the **exposure module** in which exposure levels in various environmental compartments are quantified via the modelling of the fate and distribution of the substance.
- **Effect assessment:** in the current version of EUSES it is possible to derive PNECs (Predicted No Effect Concentrations) based on the outcome of ecotoxicological studies (e.g. LC50, NOECs) provided as input. ECHA has developed a PNEC calculator as a plug-in to IUCLID6 currently for the REACH purposes. The current version of the PNEC calculator does not yet covers all the PNECs but it will be extended in the future. Therefore, it is suggested not to redevelop such a functionality in the new EUSES and limit the effect assessment module to the input of PNECs for the various protection targets. If there will be a need to use the PNEC calculator from EUSES, a solution to connect EUSES to the PNEC calculator should be sought.
- **Risk characterisation:** the risk characterisation for the various protection targets consists in comparing the exposure levels (PECs) to the PNECs. There is no plan to change this in the short term.

4.1.1. Release module

The releases for Biocides are described in the Emission Scenario Documents (ESD) for most of the Product Types (PT) and in the technical agreement for biocides TAB⁸.

In EUSES the **release rates** (in kg/day or kg/year) is the key output of the release module and the starting point for the exposure module. EUSES supports estimating release rates which can also be provided directly as set values. The release rates can be estimated in two ways:

1. Using a tonnage and a release factor:

$$\text{Release rate (kg/day)} = \text{release factor (\% or kg/kg)} \times \text{use tonnage (kg/day)}$$
2. Via various models implemented in the ESDs (for biocides), so called "consumption based approach"

For the "tonnage based approach"

- The total tonnage per use is to be reported. The tonnage used in the region and tonnage used as a site are then estimated either by default using the *fraction of the main source* and the *number of emissions days per year* from B-Tables of the TGD (EC, 2003⁹) or by overwriting those defaults.
- The current default release factors incorporated in EUSES originate from the A-Tables of the TGD (EC, 2003). It is also possible to overwrite those default release factors.
 - For REACH the agreed default release factors are now ERCs (see Annex 1 in Guidance R16).

⁸https://echa.europa.eu/documents/10162/20733977/technical_agreements_for_biocides_en.pdf/4280fd-c4-dfb0-405e-898e-70f3cdf62ce2

⁹Technical 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).

- A number of SPERCs (Specific Environmental Release categories) are developed by industry sectors, providing specific release factors to specific activities under some conditions of use. In order not to duplicate the implementation in Chesar, the SPERCs may not be implemented in EUSES but the release factors or release rates obtained from SPERCs may be used as input.

The estimation of release rates from consumption/application rate may for example use treatment areas and volumes, or use rate, such as:

- dimensions of external façade (range of scenarios) for the outdoor use of masonry/wood preservatives/paints;
- area treated (crack & crevice, barrier treatment, ant nest etc.) for indoor and outdoor use of insecticides;
- quantity used per person per day for the consumer use of disinfectants/personal care products.

4.1.2. Exposure module: fate and distribution models

The following exposure estimations are supported by the exposure module

- Local concentrations: The exposure targets are assumed to be exposed in the vicinity of the release point. The module includes various models for distribution within the receiving compartments and for the further fate and distribution in subsequent compartments. The fate in a biological Sewage Treatment Plant (STP) is modelled by SimpleTreat
- Regional concentrations: concentrations of substances released from all¹⁰ sources in a larger area (generic regional environment). The model for the fate of the substance at the regional scale (SimpleBox) differs from the model for the fate at the local scale, mainly taking into account that more time is available for transport and transformation processes.

The regional concentrations are used as background concentrations in the calculation of the local PEC. This is to account for the fact that the local environment receives not only releases from the local source but is also exposed to all the releases taking place in the region

5. Proposed scientific evolutions of EUSES

The organising committee for the workshop has drafted a number of proposals for modifying the current version of EUSES. Those are listed in the table below and are further described in Annex 2 to this document.

For each topic, a description of the proposed change and why such a change has been suggested is provided. Also an assessment of a level of priority has been made and a suggested priority is provided.

This assessment of the priority takes into account

- whether sufficient analysis/development/testing of the topic has been done so that it would be "ready" for implementation in the short term. If a topic is not "mature" enough then it will be for consideration in the long term (= not ready for implementing yet). Note that also considerations have been made of the need of the change in the regulatory context or the level of acceptance of the proposed change in the regulatory context.
- how important the change is from the business perspective (will it have a large impact on the exposure? will it impact many substances? etc.)

In summary, the "priority" is reported as being ":

¹⁰Releases from all routes to each environmental compartment for each use are taken into account.

- ready & high importance
- Ready & low importance
- Not ready & high importance
- Not ready& low importance.

Ready & high importance means that it should be considered for the first version of EUSES while *not ready & high importance* is to be considered in a future version¹¹ (as for example further research or validation is needed); the *ready & low importance* may be implemented depending on the cost for implementation and for the *not ready & low importance* it will have to be decided whether it is worth clarifying the requirements. .

A number of more detailed criteria have been used and are described in annex 2 for each topic.

The following criteria mainly impact on whether a topic will be proposed for “ready” or “not ready”

- Maturity: is the topic scientifically documented or is further research needed?
- Implemented into any IT tool?
- Regulatory considerations: to identify whether the proposal has already been agreed within for the implementation of one of the regulations.
- New data requirement: whether the input data which would be needed to estimate the exposure is usually not available

The following criteria impact on the importance from a user perspective (high or low):

- Number of assessment benefiting (e.g. based on type of chemicals affected)
- Expected impact on exposure

Note that for each topic which will be considered as ready and important, a “sensitivity analysis” should be conducted to better understand the impact of the change proposed.

¹¹ Nevertheless requirements which are seen as a high priority, even if not ready for implementation should be described as far as they can as they may impact on the architecture of the application when it will be redeveloped.

Table 1: Table listing a number of proposal from the workshop organising committee (details on each topic are provided in Annex 2)

	#	Topic	Description (proposal)	Why is it important?	Suggested priority
SUBSTANCE	1	QSARs for Koc, BCF	Alternative options to be discussed: <ol style="list-style-type: none"> 1. Keep the current implementation 2. Limit use of QSARs to cases where Koc/BCF are not information requirements under REACH or Biocides and are needed to run EUSES .Different equations are proposed for neutral organic and ionisable chemicals for the Koc. 3. Enable use of improved QSAR tools 	<p>If the selection of the QSAR for estimating the Koc is not well done, the outcome of the calculations may not be adequate. Koc could vary substantially for ionising substances if only Kow is taken as a parameter for the calculation (pKa is needed in this case).</p> <p>In addition, if any of the QSARs are applied on substances which are not well represented in the training sets of the model, the error of the calculation for both BCF and Koc can increase substantially.</p>	ready/ high importance (Option 2 preferred) as it is the most cost efficient)
RELEASE	2	Overview of “release scenarios” and proposal to revisit the current approach for designing the release module	<ul style="list-style-type: none"> • Enable the use of some of the release scenarios developed for biocides for assessments under REACH • Streamline the implementation of the various release scenarios. Systematically distinguish between i) the release estimation and ii) the exposure estimates in the receiving compartment (change UI so that exposure (PECs) currently included in the release part are available in the exposure part) 	Increase synergy, consistency across regulatory areas as well as rationalisation of IT programming	Not ready but analysis is high priority
	3	Release module	<p>Implement ERCs release factors. This also implies a change in the way to describe uses (need to introduce the various life cycle stages as in R12) and calculated default tonnage.</p> <p>Adding ESDs, and sub scenarios not yet implemented in EUSES to the existing ones and modifying some of the existing ones.</p>	<p>Align with R16</p> <p>Align with Biocide guidance and ESD calculation sheets.</p>	Ready/ high importance
	4	Addition of new release scenario <i>Direct releases to agricultural soil</i>	Add a possibility to estimate exposure from direct release to agricultural soil	Extend the applicability domain of EUSES. Such scenarios are needed under REACH (e.g. fertilizers, co formulant of pesticides, etc.)	(nearly) ready/medium importance
	5	Addition of new release scenario <i>Releases from reservoirs</i>	Allow to correctly calculate the local PECs for air and water when there is a continuous release to air and an intermittent release to water due to collection of wastewater	Such scenario has been identified as missing by the ENES SPERC working group.	Ready/low to medium importance

STP	6	Update of SimpleTreat	Replace the current SimpleTreat version implemented in EUSES by the new version SimpleTreat 4.0 with few modifications which had been agreed in BPC environment WG	More up to date modelling for the functioning of a biological STP. Aligns with Biocide guidance	Ready/ high importance
	7	Sewer Removal/(Bio)Degradation	It is proposed that the sewer model is constructed flexibly such that it can cover several removal processes by implementing a correction factor (% removed in sewer – with the default being zero)	Sewer degradation is a significant removal process for chemicals disposed down the drain.	Ready and high importance for ECETOC, ECHA considers that more discussion is needed on the boundaries of the proposal.
AIR	8	Site specific assessment	Implementation of flexible OPS model for air exposure and deposition developed by RIVM in EUSES	For site specific assessments. Various approaches based on similar Gaussian models are already currently used by applicants for authorisation, but they have to carry their calculation outside EUSES.	Technically ready (but impact to be still assess) /medium importance
	9	Air deposition of very volatile substances	From calculations done with the EU TGD spreadsheet version it appeared 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 under item 823 in 2011.	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 for volatile chemicals and substances with higher air-water partitioning coefficients. It also affects man via the environment exposure assessment.	Not ready /Important
	10	Episodic rain	EUSES (distribution part according to Simplebox 3.0) assumes constant drizzle which is unrealistic. Modelling episodic rain improves the precision between steady-state and complex dynamic models.	Standard multi-compartmental box model approach fails to correctly predict atmospheric fate of atmospheric fate of highly soluble chemicals. Considerably lower concentrations in air and higher concentrations in soil and water would be predicted for the regional scale.	Ready/Low importance
	11	Assessment of photolytic degradation	Procedure allows to estimate photodegradation half-lives under field conditions for the aquatic environment	Offers the possibility to evaluate the influence of photodegradation on persistent but only photolytically degradable substances. Method will be supportive for the persistency assessment	Technically ready (model exists) /Low importance

SOIL	12	Providing a new concentration in soil for indirect release: PEC soil initial	Allow to calculate a PEC soil right after the last sewage sludge application (PEC soil initial) in addition to the PEC soil average over a period of 30 or 180 days after the last sewage sludge application.	Align with Biocide guidance.	Ready/High importance (for biocides)
	13	Correct implementation of the depth-dependent concentration calculation in soil	Depth dependent concentration is already included for regional scale. Implemented according to previous SimpleBox version. New Simplebox version 4.0 is available with adapted implementation of soil depth. Should be introduced for the local scale and updated for the regional scale in EUSES.	More realistic assessment of the process rates from soils such as volatilization and leaching.	Ready /High importance
SEDIMENT/Water	14	Different Kp(susp) and Kp(sed) for seawater and freshwater	allow entry of separate Kp values for marine and freshwater environments	To reflect better behaviour of ionisable substances and metals in two water compartments. Improvement of calculation PEC marine water and PECsed marine water	Option 1: Ready high priority (low effort) Option 2: not ready low priority
	15	Modification of calculation of PEC sediments (REACH)	The PEC local sediment should be calculated as the Clocal_sed + PECreg_sed and not applying directly the partitioning method on the PEC water.	To enable the use of measured data for the Clocal or the PEC regional for sediments.	Ready/High importance
	16	Nested local scale multimedia model	Add multimedia transport and mass balance also at local scale (now they are taken into account at regional only) with 2 options: i) adapt the current 2 compartment local models (e.g. water-sediments) introducing mass balance concept or ii) update local exposure with the "nested" local scenario as implemented in Simplebox 3.	To estimate more accurate PECs in those cases where, for example, the mass balance matters. Potentially to include exchange mechanism (e.g. volatilisation from soil, run off and drainage to surface water) for local concentration calculations. Some of these mechanisms are taken into account in the release scenarios proposal.	Technically ready but impact may be non desired
MVE	17	Man indirectly exposed via the environment.	The proposal is to replace the calculations for the concentration in plant leaves, root crops and meat and milk. The new proposals are mainly valid for neutral organic compounds, as the current model. For plant leave the proposal consists in to modify the equation to estimate the Transpiration Stream Concentration Factor from the Kow. For the root crops the proposal consists in modifying the	Important for man indirectly exposed via the environment: The concentration in plant leave is possibly underestimated with the current model. Due to the effect of growth dilution EUSES overestimates root concentrations.	Ready/Important

			<p>model implemented in EUSES with a more recent model</p> <p>For concentration in milk and meat the proposal consists of replacing the current regression equations by a mechanistic steady state model for bioaccumulation</p>	<p>Updating EUSES with this proposed method is important because it predicts different bioaccumulation behaviour compared to EUSES.</p>	
	18	Man via the environment: alternative model for crop exposure pathway	<p>Facilitate the possibility to calculate concentrations in roots, leaves, grass (for further exposure estimation in milk and meat) for exposure of man via the environment, on the basis of transfer factors from soil to those compartments.</p>	<p>To enable to calculate MvE in EUSES for inorganics/metals. Highest need under REACH authorisation process</p>	<p>Ready/high importance for metals</p>
Sec pois	19	Secondary poisoning	<p>Addition of a new/extension of terrestrial food chain, by adding top-predators</p> <p>Addition of predatory fish in the aquatic food chain to account for additional biomagnification.</p>	<p>Those food chains are not yet accounted for in EUSES.</p> <p>Also the exposure in fish will impact on the indirect human exposure.</p>	<p>Not ready /medium importance</p> <p>Not ready/high importance</p>
Particulates	20	Nano materials (chemicals in solid state/ particulates)	<p>Adding an exposure assessment model specifically for nano materials (to be possibly later extended to particulates e.g. micro plastics)</p>	<p>Standard EUSES cannot adequately model environmental fate and exposure of nano materials/particulates</p>	<p>Technically ready with respect to fate modelling of nanomaterials at regional scale. Not ready for implementation / High importance</p>
	21	Release and fate of sparingly soluble chemicals	<p>Enable EUSES to consider in the exposure estimation the dissolution of solid substances.</p> <p>This particularly affects substances emitted in solid form, particularly metals</p>	<p>To reflect more realistic exposure estimation in water compartment. Accounting for slow dissolution could lead to lower predicted concentrations in water and higher concentrations in (the solid phases of) sediments.</p>	<p>Not ready /low importance</p>
Metals	22	Extended regional (and local) exposure model for metals	<p>Allow to calculate regional PECs after a surveyable time period (e.g. 10 years, 100 years in case steady-state is not reached) or at least indication when e.g. 95% of steady-state is reached.</p> <p>Alternatively, add long-term mineralization/immobilization processes for metals to improve steady-state local and regional exposure estimation</p>	<p>High overestimations of steady-state exposure (regional for REACH and local for some ESD) when steady-state is only reached after thousands of years (mainly sediment or soil)</p>	<p>Option 1 Ready/ High importance for metals</p> <p>Option 2: Not ready</p> <p>High importance for metals</p>

	23	Bioavailability of metals	To implement the estimation routine for metals, which reflects their behaviour (consideration of the truly dissolved phase - free ion species and inorganic complexes).	In the current version of EUSES QSARs are available to estimate substance`s partition coefficients. This mathematical routine (based on log Kow) is however only applicable for organics while for metals EUSES should be fed with the measured Kp values. If the experimental data are not provided the existing QSAR routines in EUSES will result in high overestimation of the metals (bio)availability.	Not ready/ High importance for metals
	24	Introduce natural (pristine) concentration for inorganics	To implement natural/pristine concentrations (also for biocides)	To reflect the actual "rules" of assessment for natural substances (added risk approach and total risk approach)	Ready/high importance for natural substances
Parallel/aggregate	25	Parallel assessment (for multi-constituent substances and for substances transforming on use/ in STP)	Support the parallel assessment of several constituents/substances as well as the parallel assessment of substances and transformations products. This is already possible with the Hydrocarbon Block Method in EUSES which needs to be extended to biocides.	To enable the parallel assessment of i) constituents of a substance/mixture or of ii) substances and their transformation products (or precursor and substance) Note that in Chesar it is also already possible to run parallel assessment of parent and metabolite when formed upon use or in the STP, both at local and regional scale. Distinct sets of phys chem and degradation rates have to be provided using the assessment entity functionalities, as well as an assumed fractions of parent and metabolite (or constituents/substances)	Ready/ High importance
	26	Assessment of substance transforming in the environment	It should be explored whether a more sophisticated regional model should be implemented for substances transforming in the environment. This proposal has been made based on the initial input in the RIVM report. Nevertheless clarification is needed.	Need to expend the current regional model for substances transforming in the environment to be explored	Not ready
	27	Aggregate local exposure assessment (biocides)	Support to quantitative aggregated exposure assessment covering a number of product types (PTs) with identical emission routes	There is the need for biocides to perform such quantitative aggregated exposure assessment at the approval stage of the biocidal active substance. For REACH Chesar supports the assessment of the sum of all widespread uses. Additional functionality to support the sum of local exposure could also be implemented in Chesar.	Nearly ready /High importance for biocides according to ECHA (reservations from ECETOC)

Annex 1: Stakeholders involvement in EUSES update and development process

The update of EUSES is an important activity that requires the buy-in of all stakeholders, preferentially at the different stages of the process. This should start at the level of requirements of what should be improved as well during the stage of development of the improvements. This should cover the specification of the required improvements, the testing of the improvements and ultimately the drafting of the manual.

Therefore a broad participation and involvement of stakeholders is needed, covering all users and potential contributors. There is the need to get a buy-in from industrial stakeholders that will use the tool in future updates of their dossiers and/or creating new dossiers under different legislations, but as well from authorities, not only at European level but as well at the national level where the tool is used. Transparency is needed to get an acceptance by all stakeholders, hence it is necessary to reflect how other stakeholder organisations and academia can contribute in the process. It is clear that the stakeholder engagement has to cover the different legislations that will benefit from this improvement, being industrial chemicals (REACH), biocides and probably pesticides and fertilisers. Throughout, it will be essential to ensure that reasonable timelines are established to allow for review as well as collecting and collating comments by these stakeholders.

In order to facilitate stakeholder engagement, it is proposed to establish three types of forum group, each with different remit (and potentially, participation); a broad **Expert Group**, a smaller **Preparation Committee** and, where necessary, targeted **Topic Groups**.

The **Expert Group** will act as a sound board comparable to a partner expert group for guidance documents. This expert group should cover not only the different stakeholders (authorities, industry, interested stakeholders including academia) but also the different legislations that are intended to be served by the improved tool. In order to get the appropriate participation, RAC, BPC and CARACAL should be informed, as well as EFSA and DG JRC in order to have a broad support for the Expert Group members. At the least, the broad expert group should be informed via e-mail on the different steps and the progress made, in order to get an easier buy-in at the end of the project. This expert group can be formed after having sent a description of the project to the above mentioned addressees. Preferentially, members of this expert group should engage for the period of the project. They are not expected to contribute to the real developmental work. Further reflection is needed how academia can engage in the group. The expert group could be set up after the work shop in June, but will not become really active before the pre-study has been finished.

A smaller **Preparation Committee** will be needed to decide on the most appropriate moments to inform the Expert Group on the progress made and to get the buy-in where needed to facilitate the acceptance at the end. This Preparation Committee should be the link between the developers and the expert group and the ultimate broader group of users of EUSES. This group will work via e-mail, webex and face to face meetings where needed. They can be seen as the ambassadors of the project. This preparation committee is a kind of continuation of the organising committee for the June workshop.

Since this is a longer-term project, it may be of interest to report on the progress, not only to the Expert Group, but even more broadly to scientific communities like for instance SETAC, or at the appropriate level within concerned authorities as well as the OECD. Further discussion will be needed on how to organise this and how to perform the secretarial aspects in the best way, with the potentially highest buy-in from all stakeholders.

An output from the June Workshop will be a list of topics that will be proposed to be included in the ECHA feasibility study. Each of these topics will be assigned a proposed priority. Following the workshop there will be an opportunity to express interest in joining a specific **Expert Topic Group**. The Expert Topic Group will provide the opportunity to explore technical aspects related to the topic issue in detail. In the first instance the Expert Topic Groups will review the technical input to the pre-study, since technical aspects may influence the feasibility and, hence, priority that is assigned to the topics. Once the full EUSES update project is launched, the relevant

Expert Topic Groups will be consulted on any technical decisions required and will perform focused testing of relevant aspects of the beta versions of the IT tool.

It is recognised that the number of Expert Topic Groups may become unmanageable, due to the large number of topics. Hence, topics will be grouped together. The groupings will be decided on the basis of webex as necessary to discuss key points. The preparation committee will provide oversight of the Expert Topic Groups and they will be set up following the workshop.