

## Release note Chesar 3 (and migration tool)

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## 1. Known issues

### 1.1. Helptext

In internet explorer 11, the display of the helptext does not yet work conveniently. If you have opened the Chesar on-line helptext, when pressing a new helptext icon, the helptext window is hidden (behind Chesar). You should fetch it yourself. Alternatively always close the helptext window once read.

### 1.2. Import from IUCLID

For ensuring full compatibility with IUCLID 6 you need to update your IUCLID 6 installation with an updater that will be available on 21 June 2016 on IUCLID website. (<https://iuclid6.echa.europa.eu/>).

The values shown for the PNECs and DNELs imported from IUCLID are displayed with 2 digits, and therefore look as if rounded. Nevertheless the RCR are calculated with the precise number.

When re-importing a substance from IUCLID 6 into Chesar 3, the molecular weight used for the assessment is systematically recalculated, even if no change has been made in IUCLID. Therefore, if you had manually provided the input, you will need to re-type it again. You can see the previously entered value in the synchronisation message.

The import of IUCLID 6 legal entities in Chesar box 7 cannot be performed. However, IUCLID 5 legal entity files (.i5z) can be correctly imported.

### 1.3. Exposure assessment workers


TRA Workers: Exposure estimates are provided when *Place of use* is set to "Indoor and outdoor", although the tool should not provide an estimate for such setting.

When you delete a main exposure dataset, no RCR is calculated until a new exposure dataset is set to main.

### 1.4. Environmental assessment

The total releases are not displayed in the exposure from *aggregated sources* tab (as they were in Chesar 2).

When changing the tonnage for a use at industrial site in Box 2, the daily and annual use amount at site (in the contributing scenario in Box 3) is not updated although a warning message says it is

 The local tonnage for the environmental contributing scenarios in Box 3 will be recalculated by default. If you had reported specific values you should manually report them again.

. If the amount at the site were calculated by default you may trigger the recalculation of the default values by removing the existing numbers.

The "Local release rate" is not shown, if the release after on site RMM is 0.

When the releases to the environment are based on ERCs, the defaults provided in Chesar for ERC 8c and ERC 8f are not in line with the latest version of the guidance on environmental exposure assessment R16 ([http://echa.europa.eu/documents/10162/13632/information\\_requirements\\_r16\\_en.pdf](http://echa.europa.eu/documents/10162/13632/information_requirements_r16_en.pdf)). You should therefore manually modify the values, by using the release estimation method: **Estimated release factor** for water and adapting the values according to R16, as shown below.

ERC		Release		
		to air	to water (before STP)	to soil
8C	Widespread use leading to inclusion into/onto article (indoor)	15%	30% (1% in Chesar) The default release factor of 30% applies to activities/processes where the substance is dissolved/dispersed in a surplus of water and applied to an article via dipping/immersion or spreading (e.g. textile dyeing/finishing or application of polishes with floor cleaning water). For other widespread uses (e.g. use of paints and adhesives, including water based products) the release factor of 5% is applicable.	n.a.
8F	Widespread use leading to inclusion into/onto article (outdoor)	15%	5% (1% in Chesar)	0.5%

When changing the Setting for the *Release percentages of modelled biological STP* in Box1, the values are used by default for the "standard biological STP" in the assessment in Box 3, but when setting the biological STP to "site specific" those values are not used by default. The "Site specific" release percentages should then be manually checked and provided.

Also the specific *Release percentages of modelled biological STP* from Box1 are not considered for the calculation of the regional PEC.

## 1.5. CSR generation

When generating the full CSR see the release note of the CSR report generator, available at [http://iuclid6.echa.europa.eu/documents/21812392/22308511/IUCLID\\_6\\_Release\\_Notes\\_1.0.0.pdf](http://iuclid6.echa.europa.eu/documents/21812392/22308511/IUCLID_6_Release_Notes_1.0.0.pdf).

## 1.6. Exposure scenario for communication

In the short title, the order in which the PC, SU and AC is provided is not fixed


The local release rate to soil is systematically displayed in section 3 of the ES for SDS, although it is not taken into account for exposure estimation at the local scale by EUSES, and consequently it is not displayed in the user interface of Chesar.

The rounding of numbers in the ES for communication is not the same compared to what is printed in the CSR and what is displayed on the screen.

## 1.7. Complex cases

The order of assessment entities as entered in IUCLID, is not kept when importing substance information from IUCLID 6.

## 1.8. For beta testers of Chesar 3

 Note to the beta testers of Chesar 3:

You should **never reuse data** generated with the beta version of the migration tool or beta version of Chesar 3.

Also you may encounter user interface issues (including logging in difficulties) if you have used a beta version of Chesar 3. To fix it, delete your browser's history.

## 2. Changes to existing features or new features

### 2.1. Editing and saving

#### Direct editing in Chesar.

In Chesar 3 inputs can sometimes be changed directly by typing in the application. They are immediately saved as soon as you click somewhere else in the page. There is no undo button.

#### Remember to scroll down the Chesar page to find the save / cancel buttons!


In Chesar 3 inputs need sometimes to be actively saved (or cancelled). In this case one of the two button **save** or **cancel** need to be clicked. Be aware that these 2 buttons




are at the bottom of the pages and not always visible. So remember to scroll down and save your work! For example, if in box 2 you modified a contributing activity / scenario (forgetting to click on save) and you click on another contributing activity/scenario in the tree, the information you entered will be lost.

#### Remember to scroll up if you cannot save the page!

If nothing happens once you pressed **Save** it may be because some information is missing in one of the fields. Such information will be identified by a red message (e.g.

• Tool version is required ).

### 2.2. Helptext

In a number of screens you will see a  which indicates that some helptext specific to that view is available. We highly recommend that you have a look at those helptext which provides instructions on the various functionalities available in the tool. (see also 1.1 **Error! Reference source not found.** for known issues with internet explorer 11)

### 2.3. Communication with IUCLID 6

#### 2.3.1. Webservice functionality

In Chesar 3 the interaction with IUCLID 6 is done by using webservice in a much easier way than what was implemented in Chesar 2. However, in Chesar 3 it is not anymore possible to simply import a IUCLID export file. Therefore, to start the assessment of a new substance or to synchronise your substance data in Chesar with the data in IUCLID, you need a IUCLID 6 installation to which to connect via the webservice.

#### 2.3.2. Change during import/synchronisation

In Chesar 2, when importing a substance, the lower bound of the molecular weight (MW) reported in section 1.1 was taken into account for the assessment (mainly for exposure estimation by EUSES and ECETOC TRA workers). In Chesar 3 the range of MW is imported, when available. The upper bound of the range is taken as default for exposure estimation (see 2.4), as this is more conservative for estimating the exposure to workers with ECETOC TRA. If a substance was already in Chesar 2 and is migrated from Chesar 2 to Chesar 3, the MW used for the assessment is the one which was available in Chesar 2, i.e. the lower bound. If the substance is reimported from IUCLID, synchronisation will occur and the upper bound will be used for the assessment if available. As a consequence, the exposure estimates will be recalculated. Therefore you are advised to systematically re synchronise your substance data between IUCLID and Chesar (by re importing your migrated IUCLID 6 dataset to Chesar 3) when starting to work on your assessment for the first time in Chesar 3.

### 2.4. Properties of the substance: molecular weight used for the assessment

It is now also possible to manually set a value for the molecular weight to be used for the

assessment. By default this value is set to the upper bound, if available, of the range provided in the reference substance in IUCLID, otherwise the lower bound. Note that for assessment entities being a group of constituents, the "molecular weight for assessment" is the arithmetic mean of the MWs of the various constituents.

## 2.5. Exposure assessment: exposure scenario building and CSR generation (Box 3 and Box 4)

In Chesar 3 the full exposure assessment is carried out in Box 3, including the qualitative assessment. The starting point is the contributing scenario (CS) which contains all the conditions of use assumed. You have to select how the conditions of use are defined for the CS. They may be based on

- SPERCs for the environment
- SCEDs (or ECETOC TRA subcategory) for consumers
- SWEDs for workers (in future).

Alternatively they can be "manually entered", and this can be done in two ways:

- Select conditions of use from the library (Box 6)
- Create a TRA exposure dataset (either for the whole life cycle by *Adding default exposure dataset*, or for the single CS by *adding a new exposure dataset*). In this case all the input parameters to the TRA are included in the CS (as conditions of use).

You can use exposure estimates for your assessment either automatically calculated by ECETOC TRA or by EUSES, or manually reported for measured data or data obtained with other exposure estimation tools. It is up to you to ensure that the exposure datasets are consistent with the conditions of use described.

You may press the "validate assessment" button to see, for example, why no exposure estimates are provided.

In Chesar 3, Box 4 is only used for completing the CSR and generating it.

## 2.6. Environmental assessment

The setting of the modelled biological STP have been made flexible in Chesar 3. The fractions emitted to the various routes (air, water, sludge) and the fractions degraded in the biological STP are still calculated by default by SimpleTreat in EUSES, as in Chesar 2. However, you can change now those default values in Box 1 (tab *Fate in standard biological STP*), and this would apply then to all contributing scenarios for the environment by default (instead of the SimpleTreat defaults). You can also change the default values by setting the Biological STP to "site specific" in a single contributing scenario.

It is now also possible to manually carry out the assessment (and report it), based on environmental concentrations measured or obtained from external tools.

An additional new feature is the possibility to flag a use as being a "use under rigorous containment with minimisation of releases". The information will be reported in IUCLID when the uses are exported, and can be taken into account by the authorities for de-selecting/deprioritising substances for further regulatory action.

### 2.6.1. SPERC

The SPERC format (Box 6) has been modified, based on the input of the ES/CSR roadmap SPERC group and a number of changes have been introduced:

- The conditions of use are reported at SPERC level (in Chesar 2 it was at subSPERC level). This is because the conditions of use for a contributing activity apply to all substances in that use (e.g. in a type of mixture), irrespective of the single substance assessed. It is the release factors that may differ for the various substances part of a mixture. As in Chesar 2, subSPERCs within a SPERC enable to provide differentiated

release factors for the various substances in the mixture when relevant. You will have to select the appropriate subSPERC for your substance.

- It is not possible anymore to include within a SPERC "Optional risk management measures". When using a SPERC a registrant is expected to stick to the set of conditions of use described in the SPERC and the related release factors (before biological STP). When using a SPERC in your assessment you can only modify the values for the following conditions: amount, setting of biological STP and dilution in the receiving environment, as they do not impact on the release factor provided in the SPERC.
- The explanations for the releases can be reported either at SPERC level (valid for all subSPERC to prevent duplication) or at subSPERC level
- It is possible to flag that a SPERC describes a release to agricultural soil.

## 2.7. Human health assessment

For the assessment of local dermal and eye effects, it is possible to report a concentration limit of the substance in mixture in Box 1 (tab *Hazard conclusion and scope of assessment*, Workers and Consumers), below which no effects to skin and eyes are expected to occur. Usually this corresponds to the classification threshold for mixtures. For the contributing scenario where the *percentage of substance in mixture* is set below such concentration limit, the tool will consider the risks as being controlled for those effects.

It is possible to add, delete or edit conditions of use in several contributing scenarios in one go (bulk actions in Box 3).

Note that when deleting an exposure dataset, the conditions of use linked to that particular dataset are not deleted automatically as well. They can be deleted one by one pressing the delete button next to them.

Also note that when adding a new exposure dataset, this is by default set to "main", even if you already had a main assessment (which consequently becomes "supportive"). You have to set the final status (Main/Supportive) in the exposure view.

### 2.7.1. ECETOC TRA workers

For liquid substances, the exposure estimate by inhalation is based on the vapour pressure at operating temperature. In Chesar 2.3, the vapour pressure as reported in IUCLID (usually at 20°C) was used. In Chesar 3, the vapour pressure at operating temperature up to 40°C (default operating temperature in Chesar) is automatically recalculated (but you can overwrite it). Therefore the inhalation exposure estimates may be different than the ones you were used to in Chesar 2.

In Chesar 2 all the inputs to the ECETOC TRA workers were provided as determinants (conditions of use). In Chesar 3 it is the same except for

- *LEV for Dermal: Yes*
- *vapour pressure at elevated temperature*

These two inputs are considered to be exposure estimation assumptions rather than conditions of use. Consequently they are now treated as *TRA Workers specific parameters*, which can be accessed by editing the TRA workers exposure dataset. Those assumptions will be reported in the exposure section in the CSR.

In addition a new possibility to limit the inhalation exposure to the saturated vapour concentration of the substance has also been implemented, as suggested by the ECETOC TRA manual. This is also to be set in the *TRA Workers specific parameters*.

For solids for which the operating temperature is above the melting point, the exposure estimate is, like for liquid, based on the vapour pressure at the operating temperature.


## 2.7.2. ECETOC TRA consumers

The TRA consumer 3.0 (the version in Chesar 2 supporting the exposure estimation for TRA subcategories only) and version 3.1 (the version in Chesar 2 supporting the use of SCEDs) have been merged into one single version. You have to decide at the beginning whether the assessment is based on TRA subcategories, SCEDs or manually entered information, and then the TRA consumer 3.1 algorithm<sup>1</sup> is applied consistently to those conditions of use.

As a consequence of the harmonised application of TRA consumer 3.1 algorithm to SCEDs and to TRA subcategories, there will be discrepancies for four PC/AC subcategories between exposure estimates obtained using the ECETOC version of the TRA and the version of the TRA implemented in Chesar 3: the dermal exposure estimate for PC12 "Lawn and garden preparation", AC5 "Clothing (all kind of materials), towel", AC5 "Bedding, mattress" and AC8 "Printed paper (papers, magazines, books)" is higher in Chesar 3 compared to ECETOC TRA. This is due to a difference in data structure between SCED and TRA subcategories. In the SCED, the selection of *adult* or *child* as a target group impacts on the exposure for all routes in the same way. In the four particular ECETOC TRA subcategories mentioned above, the exposure is instead estimated on adult parameters for some route and child for other route. In Chesar3, the TRA has been implemented with a data structure consistent with the SCED data structure. As a consequence, for the above 4 subcategories "child" has been selected by default for the assessment (as being the most conservative leading to a higher exposure estimate for the dermal route than in ECETOC for that subcategory).

## 2.8. CSR generation and export to IUCLID

Box 4 now only relates to the generation of CSR. In the left hand side you can see the table of content of the CSR. You will find more information in the Chesar helptext for Box 4.

Note that most of the explanations for the CSR have to be reported by the assessor in text fields identified in the application (box 1, 2 and 3) by the following icon .

Note that the export of use and exposure information to IUCLID and the generation of the full CSR can only work if you have IUCLID up and running

Also, when exporting your uses to IUCLID, Chesar and IUCLID data have to be synchronised. The first time Chesar will systematically request you to reimport your data from IUCLID 6, if you did do it already with Chesar 3. This is because two new fields are imported from IUCLID (upper bound of molecular weight and extrapolation method for the PNEC derivation).

## 2.9. Assessment entities: assessment of "complex cases"

Chesar 3.0 supports the assessment for the following types of substances:

- Substances with several compositions having different hazard profiles (e.g. due to impurity)
- Substance transforming on use or in the environment
- Multi constituent substances where (group of) constituents behave differently

For that a functionality has been implemented for i) assigning the relevant assessment entities (defined in IUCLID 6) to each contributing scenario and for ii) supporting parallel exposure assessment of those assessment entities for each single contributing scenario

## 3. Migration from Chesar 2.3 to Chesar 3.0

Most of the data available in Chesar 2.3 will be migrated to Chesar 3.0. The release/exposure estimates which are the results of a calculation within Chesar will be recalculated during the migration. In few cases explained below the calculations may lead to a different result than what it was in Chesar 2.

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<sup>1</sup> TRA 3.0 algorithm is not implemented in Chesar 3



## 3.1. Situations where exposure estimates are expected to be different in Chesar 3 compared to Chesar 2

### 3.1.1. ECETOC TRA workers

TRA workers exposure estimates for inhalation for liquid substance may be different in Chesar3 compared to Chesar 2, if the vapour pressure at operating temperature falls into a different TRA volatility band than the vapour pressure at 20°C (as reported in IUCLID). See section 2.7

### 3.1.2. ECETOC TRA consumers

For 4 subcategories the dermal exposure estimates will be higher than they used to be in Chesar 2. For explanations see section 2.7.2.

In case you had made two assessments with TRA consumers for a given contributing activity (e.g. one main assessment based on SCED and one supportive assessment based on a TRA subcategory), only one will be migrated to Chesar 3.

## 3.2. What may not be migrated from Chesar 2 to Chesar 3

Some SPERC-based assessment for widespread use may not be migrated. This may be due to an incorrect selection of the SPERC for the contributing scenario in Chesar 2.: If a SPERC had been defined as relevant for consumer uses only, it was nevertheless still possible to (incorrectly) select it for assessing a widespread use for professional workers. In Chesar 3, a validation rule is implemented, and therefore assessments with incorrectly assigned SPERCs in Chesar 2 are not migrated.

The following conditions of use, which were part of TRA assessment are not migrated as conditions of use:

- *Solid in solid mixtures: Yes.*
  - As in Chesar 2, no exposure estimates are provided by the ECETOC TRA for solid in liquid mixture, as described in ECETOC manual TR114, but this is only flagged by a message by pressing the validate assessment button
  - For melted solids, Chesar 3 compares the operating temperature to the melting point.
- *Containment: (PROC dependant value, No for a number of PROCs).* For PROC 1 to 3, a new condition of use is included by default when a TRA based exposure dataset is used to take into account the containment assumed by the TRA.
- *AC or PC subcategory* when using the TRA consumers: In such case the information is migrated as identifier of the TRA subcategory selected and not a condition of use.

For conditions of use for which the *determinant types* in Chesar 2 had a text in the *Description of value for CSR*, this text is not migrated to the assessment in Chesar 3. But it is migrated to the field *Default explanation for CSR* in the condition of use template in the library of Chesar 3. This new field in the condition of use template is now used as default text in the *Explanation for CSR* field associated to the condition of use in the assessment. Therefore it is possible to get the text back in the assessment by "refreshing" the condition of use, i.e. the condition of use or its value should be removed and reinserted. Nevertheless the drawback of such solution is that the specific *explanation for CSR* from the assessment will be lost.

## 3.3. Specific migration behaviour

### 3.3.1. Migrating SPERCs in Library:

SPERCs are migrated only with the "mandatory" conditions of use (those linked to the initial release factor). Therefore the optional RMM will not be migrated.

If a SPERC contained several subSPERCs in Chesar 2 with conditions of use being totally similar across the subSPERCs, then the SPERC is migrated to one SPERC (with the different release factors for the various subSPERCs). If the conditions of use differ, then each subSPERC is migrated to a new SPERC.



### **3.3.2. Migrating SPERC based assessment**

There is one exceptional rule for the migration of an assessment based on SPERC. If there was a *RMM with effectiveness* determinant in the assessment (beside "Municipal SPT" built-in one), then, in Chesar 3, the conditions of use are reported as "manually entered" and the release estimation method will be set to "Estimated release factor" instead of SPERC. However the conditions of use and the release factors are the same to what they were in Chesar 2.