

Beta version of Chesar 3 – important information for testers

The following notes are related to the **Chesar 2016.03.21** packages.

Due to a bug during the installation of the server beta version of Chesar 3 (2016.03.08) using Oracle database, a new built is now provided. It also contains a few fixes for known issues.

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

After the testing is complete, please **delete the beta test version and data**.

Also if you have used the beta version distributed on the 8 march (Chesar 2016.03.08 version) do not reuse data from that version into the 2016.03.21 version.

2. Be aware that some **helptext** is available in the application. Click on the  when you see one. More should be available in the final version of Chesar 3. We welcome your feedback on the provided helptext: Is it useful? Is it clear?

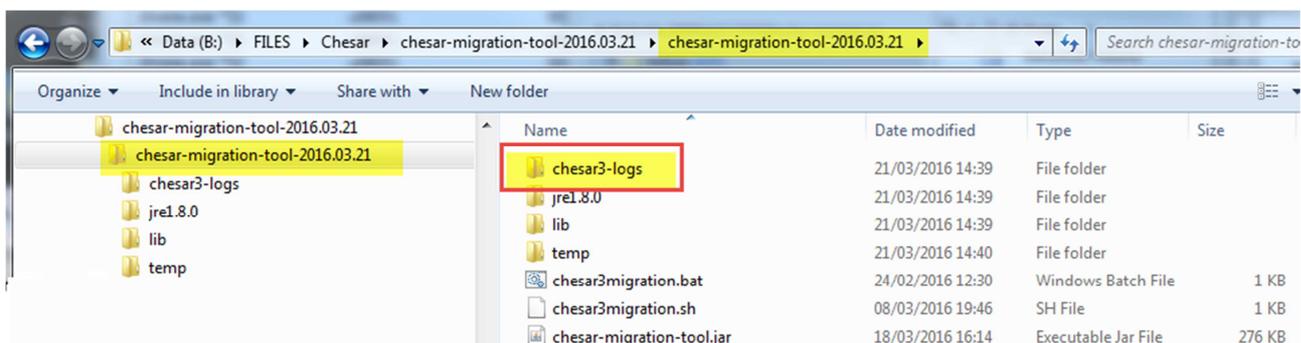
It is planned that Chesar 3 will be released together with IUCLID 6 at the end of April.

If you have a limited time to dedicate to testing, please focus the testing on:

- **Migration tool:**

- If your migration report identifies any failure or error in the migration , please send your log file to us immediately

For that please **zip** the “chesar3-logs” folder and send it to chesar@echa.europa.eu.



- Check the migration of contributing scenarios where you have used several exposure assessment (for example to cover the different routes by different tools)
- Check the migration of environmental contributing scenarios which have been based on SPERCs.

- **Beta version of Chesar 3:**

- Test the new functionalities (see section 3)
- Test the export to IUCLID 6
- Test the generation of CSR (section 9 and 10)

How to give feedback?

If you face any major issues (unexpected error or crash of the application), please send feedback immediately to Chesar@echa.europa.eu

If you want to submit your ideas for improvements, please do so in a Word document with the following format:

#	Title	Box	Description	Level of priority
			<i>Issue (description of what is the improvement expected to solve/support. Include screenshots when relevant)</i> <i>Proposed solution</i>	

Please send the document to Chesar@echa.europa.eu preferably by 8 April 2016.

We will not provide individual feedback to all the ideas but may contact some of you for clarifications.

Known issue planned to be fixed for the final release:

- The full CSR cannot be generated
- The creation of SCED report is not yet available
- Formatting of migrated explanation text to be improved
- If you export, delete and reimport your substance the explanations is not saved in Box 4 text boxes when the text is very long.

DRAFT Release note Chesar 3

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1. User interface- general

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

 Save  Cancel 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 the form. Such information will be identified by a red message (e.g.  Tool version is required ).

2. Changes to existing features

2.1. Communication with IUCLID 6

2.1.1. 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.

2.1.2. 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 and the upper bound of the range is taken as default for exposure estimation, 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. The exposure estimates will be recalculated and therefore modification will occur.

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

In Chesar 3 all 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 the way by which 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
- in the future on SWEDs for workers.

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 data set (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 and you have to set their values.

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 tools. It is up to you to ensure that the exposure data sets are consistent with the conditions of use described.

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

2.3. 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. They are usually determined by the most critical substance. Only the release

factors 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: 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
- Some fields have been renamed.
- It is possible to flag a SPERC as being relevant for a "use under rigorous containment with minimisation of releases". The information provided then in the SPERC will be reported in IUCLID by the registrant and can be taken into account by the authorities for selecting/deprioritising substances for further regulatory action.
- It is possible to flag that a SPERC describes a release to agricultural soil.

2.4. ECETOC TRA workers

Only one change impacts on the exposure estimates. For liquid substance, the exposure estimate 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 recalculated by Chesar. You can overwrite it.

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 exposure estimation assumptions, and thus they are now treated as *TRA Workers specific parameters*. Those assumptions will be reported in the exposure section in the CSR.

A new possibility to limit the inhalation exposure to the saturated vapour concentration of a substance has also been implemented.

2.5. 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 version only. 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 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 few 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 the 3 routes in the same way. In the four particular ECETOC TRA subcategories the exposure is estimated on adult parameters for a route and child for another 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). It remains possible to change the choice to adult (in which case the exposure on the inhalation/oral route will be lower than what it is in ECETOC TRA for that subcategory).

3. New features

3.1. 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.

3.2. Properties of the substance

The molecular weight is imported from IUCLID but it is now possible to select a value to be used for the assessment. By default this value is set to the upper bound of the range provided in the reference substance in IUCLID if available, otherwise the lower bound. Note that for assessment entities being a group of constituents, the “molecular weight for assessment” is the mean of the MWs of the various constituents.

3.3. Environmental assessment

The fraction emitted to the various routes (air, water, sludge) and the fraction degraded in the biological STP can now be manually modified. The default values are calculated by SimpleTreat in EUSES. Nevertheless you can change them in Box 1 (tab *Fate in standard biological STP*) and this would apply to all contributing scenarios for the environment by default, instead of the SimpleTreat default. You can also change them based on site specific information by setting the Biological STP to “site specific” in a single contributing scenario.

It is now possible to manually report and make use of measured concentration in the environment or concentration in the environment obtained from external tools to carry out the assessment.

3.4. 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).

3.5. 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

On the right side the functionality foreseen for a future version of Chesar is to have a view of the CSR where text fields could be edited. At the moment only some text field can be edited here. 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 and have set up the connection by web service.

When exporting uses to IUCLID and selecting *Remove the uses already available in your IUCLID which have no corresponding own (join) use in Chesar* only the use with no corresponding Chesar use which have a status (covered by a joint CSR/covered by an own CSR) are deleted.

Also when exporting your uses to IUCLID, Chesar and IUCLID data have to be synchronised. The first time you will do so Chesar will systematically request you to reimport your data from IUCLID if you had not done so already with Chesar 3. This is related to the import of two new fields from IUCLID (upper bound of molecular weight and extrapolation method for the PNEC derivation).

3.6. 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 be assessed to each contributing scenario and ii) supporting parallel exposure assessment of those assessment entities for each single contributing scenarios.

4. 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.

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

4.1.1. ECETOC TRA workers

TRA workers exposure estimates for inhalation for liquid substance may be different in Chesar3 compared to Chesar 2 in case the vapour pressure at operating temperature is in a different volatility band defined by the TRA than the vapour pressure as reported in IUCLID (at 20°C). See section 2.4

4.1.2. 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 2.5.

In case you had in Chesar 2 two assessments made 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.

4.2. 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 to the contributing scenario in Chesar 2. In Chesar 3 such incorrect selection of SPERC is not possible. In Chesar 2 if a SPERC had been defined e.g. as relevant for consumer uses only, it was nevertheless still possible to 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 2.0 are not migrated.

4.3. Specific migration behaviour

4.3.1. 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, if the conditions of use across the subSPERCs were totally similar then the SPERC is migrated to one SPERC with the different release factors for the various subSPERCs. If the conditions of use slightly differed then each subSPERC is migrated to a new SPERC.

4.3.2. Migrating SPERC based assessment

For assessment based on SPERC in Chesar 2.3 then the migration rule depends on the list of conditions of use (determinants) associated to this assessment:

- If the list of conditions of use in Chesar 2.3 does NOT have any RMM with effectiveness determinant (beside "Municipal STP" built-in one) then the Environmental CS from Chesar 2.3 will be migrated as "SPERC based" to Chesar 3 and will have only those conditions of use that come from the migrated SPERC.
- If the list of conditions of use in Chesar 2.3 has at least one RMM with effectiveness determinant (beside "Municipal SPT" built-in one) then the corresponding Environmental CS from Chesar 2.3 will be migrated as "Estimated release factor based" to Chesar 3.0 (the release estimation method is changed). The CS in Chesar 3.0 will have all the conditions of use that were available in Chesar 2.3 and the initial release factor is set to the release factor of the SPERC used in Chesar2. The effectiveness of all the additional RMMs are applied to the initial release factor so that the release factors are maintained.