Release notes Chesar 3.4.1

Contents

1. What is new in Chesar 3.4.1

Chesar 3.4.1 implements a number of new features, as well as changes and improvements to existing features, described below. To have the optimal use of Chesar, we strongly recommend that you upgrade to Chesar 3.4.1. The update is fully compatible and works best with IUCLID 6.3.

1.1. Alignment with IUCLID

The following format changes in IUCLID 6.3, impacting on Chesar, have been incorporated in Chesar 3.4.1:

- In the endpoint summary for Biodegradation in water and sediment: simulation tests (5.2.2) the possibility to add a half-life in freshwater as well as marine water has been implemented in IUCLID 6.3 (instead of just one half-life with the possibility to specify the type of water). These values are both imported into Chesar 3.4.1 and taken into account in the EUSES calculations, where relevant.
- If entered in the endpoint summary for Bioaccumulation: aquatic / sediment (5.3.1), the BMF in fish is now imported into Chesar and taken into account in the EUSES calculations where relevant.
- The Assessment entity section in IUCLID 6.3 has been renamed Assessment approach (assessment entities) and moved from section 0.4 to section 1.10. This change has been taken into account in Chesar 3.4.1.
- In the endpoint summary for section 6 (ecotoxicological information), for Secondary poisoning the picklist entry "no or insufficient data available at present" has been changed to "Insufficient hazard data available (further information necessary)" to align with the other hazard protection targets. Both the old and the new entry are recognised by Chesar 3.4.1.

In addition, the generation of the full CSR takes into account all the improvements implemented in IUCLID 6.3 (part B sections 1-8).

1.2. Substance management

Several changes and improvements have been implemented in Chesar 3.4.1 in relation to the management of substances in box 1:

- Direct **update** (re-import) of a substance dataset already imported in Chesar via web service. Similarly to the import process, a comparison of the values in IUCLID and Chesar is made by the tool. If differences are identified, these will be shown and you will be asked whether you want to overwrite the values in Chesar.
  Be aware that the update button will not work when you have imported a dossier or a Chesar substance (.chr3) file. In these cases, if you want to update the substance information in Chesar you will need to import the updated substance/dossier via the "Import IUCLID substance dataset via web service" button.

- In the **Adsorption coefficients** tab, a checkbox including an explanation field has been added to indicate whether your substance is **adsorptive**. In case the substance has a log Kow above 5 or in case no log Kow is available and the substance has a Koc above 1000, the substance will be assumed to be adsorptive and the adsorptive flag will be set automatically by Chesar. In this case, the explanation will be filled automatically and the flag as well as its explanation will not be editable. When the adsorption or binding behaviour is not triggered by the lipophilicity, a substance can also be manually flagged as **adsorptive**, and an explanation can be added.

When a substance has been flagged as adsorptive, if the PNECs for sediment and/or soil have been derived based on the equilibrium partitioning method, the risk characterisation ratios for those protection targets will be multiplied by a factor of 10 to account for uncertainty due to the potential for adsorption of the substance.

1.3. Use description

Several useful improvements have been implemented in Chesar 3.4.1 on the handling of the use description in box 2:

- A new button "**information on life cycle tree**" has been added. When clicking on it, a pop-up appears informing the users of any possible inconsistencies in the life cycle tree. Examples of inconsistencies reported include unexpected combinations of ERCs, missing (links to) service life or inconsistent tonnages defined.

- Chesar 3.4.1 implements some new **bulk actions** in box 2. These bulk functionalities may be particularly useful for assessors incorporating use maps in their assessment. The new **bulk delete** allows to delete several selected uses/contributing activities in one go. The **bulk edit** allows you to edit a number of fields for a group of selected uses at the same time, for instance when you import a use map and would like to complete it with some substance-specific information. The following fields can be edited via this functionality:
    - Regulatory status
    - Explanation for regulatory status
    - Technical function of the substance during use
    - Form in which the substance is supplied to the use

  Note that these fields are also transferred to IUCLID section 3.5 when you export your uses to IUCLID.

- In order to identify more clearly the fields relevant for completing the use description in IUCLID, the "Show additional fields relevant for use description in IUCLID" checkbox is now always selected for those uses where information has been entered in at least one of these additional fields. The check box is unticked when none of the additional fields have been completed.

1.4. Use map related features

1.4.1. For sectors developing use maps

Chesar 3.4.1 is now able to generate SWED reports according to the agreed .xls template. In addition, the use map report has been fixed to be further aligned with the agreed template. This facilitates the maintenance of the documentation of use maps, but also enables use map developers to check whether the information provided in the Chesar file is adequate.

When duplicating a SPERC for Professional and Consumer life cycle stages, the release section is now kept. Keep in mind the conditions of use may nevertheless differ between professional and consumer uses and may therefore need to be adjusted.

1.4.2. For users of use maps

For assessors incorporating use maps in their assessments, beside the support for bulk edition

/ bulk deletion of use map elements as described above, Chesar 3.4.1 provides increased support in case an assessor imports an updated version of a use map. When deleting any uses / CAs which are part of a use map (either one at a time or by using the bulk delete functionality), a **justification for deletion of use map Uses / Contributing activities** field will appear. Chesar will remember which uses / CAs have been deleted, together with the justification entered. Note that the justification will only be saved for uses / CAs belonging to a use map. No justification can be entered for uses / CAs which are not part of a use map. When you import an updated version of the use map, the justification entered before will be shown to help you decide whether you want to re-import the previously deleted uses / CAs.

Besides this, the "comparison" table listing all changes compared to the version of the use map already available in Chesar, as well as the related report, have been improved. The list of changes now also includes the previously deleted use map elements and the justification entered when they were deleted.

1.5. Exposure assessment

1.5.1. Environment

When use maps or CSAs are imported in a specific substance in Chesar, the SPERCs associated to these elements are now always kept, also in case of a complex substance and in case no applicable sub-SPERC matching the substance properties is available. When clicking the "exposure estimates information" button in box 3, a new message appears informing the user that a suitable sub-SPERC should be selected or, if none is available, the link to the SPERC should be removed from the assessment.

When changing from a SPERC based scenario to Manual selection while retaining the conditions of use, the releases are now set to "Estimated release factor" and the "source name" field includes a reference to the SPERC ("based on SPERC <code>"). The release factor "before on-site RMM" is backward calculated from the SPERC release factor taking into account any RMM in the set of CoU so that the final release factor before any further change is equal to the SPERC release factor. Explanations for the release fractions from the SPERC are also maintained.

Where relevant, the information on BMF in fish as well as the half-life in marine water is now taken into account in the EUSES calculations.

1.5.2. Workers

The TRA specific parameter *vapour pressure at operating temperature* (in Box 3) is now reset to the default estimated value in the following cases:

- When the operating temperature is changed (in this case only the contributing scenario(s) where the operating temperature is changed is/are affected)
- When the vapour pressure of the substance is changed in box 1 (in this case all TRA Workers datasets are affected)

This may have an impact on the exposure estimates for any datasets where you had overwritten this default value to provide a more adequate value. In this case, you will need to re-enter it (if still relevant). Be aware that the resetting of the vapour pressure at operating temperature will not be automatically undone when the vapour pressure is reverted to its original value in box 1 (i.e. the *vapour pressure at operating temperature* will not go back to its original overwritten value).

1.5.3. Library improvements

Several useful improvements have been implemented in Chesar 3.4.1 on the handling of library items in box 6:

- Chesar 3.4.1 facilitates the cleaning of library elements by allowing you to search for the "unused items". These non-relevant elements can then be selected and deleted in one go.

- It is now easier to understand which conditions of use and SPERC/SWED/SCED are set to obsolete as they are shown in italic. Moreover, when checking where a condition of use has been used, the Chesar version of the related SPERC/SWED/SCED is now also shown.
- The search has been enhanced by making some changes to the information shown and by adding the possibility to sort the search results by code and by life cycle stage (for SPERCs), PROC (for SWEDs) or PC/AC (for SCEDs).
- Chesar 3.4.1 allows the update of non built-in CoU (defined by sectors) by Chesar built-in ones.
- The dialogue displayed to the user when library elements (CoU/SCED/SWED/SPERC) are imported is now more accurate and clearer.
- Standard phrase catalogues will be treated as a whole, which means that from Chesar 3.4.1 onwards, all phrases associated to the catalogue imported will have the same versions.

1.6. Generation of ES for communication

Some small changes have been made to the structure of the ESComXML generated, to make the generated files more accurate and easier to process for recipients.

In addition, Chesar 3.4.1 displays a warning message informing the users that the section 3 will not be included in the extended SDS for a complex substance.

1.7. Generation of CSR

Small changes have been made to the generated CSR in Chesar 3.4.1, including a better description of qualitative risks and improvement of the presentation of information for PBT substances.

1.8. General

A warning message has been added when changing the **water solubility**, **log Kow** or **vapour pressure**, to warn the user that this change may lead to the removal or change of selected sub-SPERC(s) (in Box 3) if the new value does not fall within the range specified in the sub-SPERC(s). For vapour pressure, the warning also warns for possible changes in TRA workers datasets (this may the case if the vapour pressure at operating temperature has been overwritten, see also section 1.5.2 of these release notes).

Several warning messages in boxes 1, 3 and 6 have been improved and clarified. Warning messages have been added in box 3 and 6 when you leave a dataset / element without saving. Remember to click the *Exposure estimates information* button in box 3 to visualise the warnings. In addition, a warning is now shown when trying to add a standard phrase when no phrase catalogue has been imported. Once standard phrases have been entered, their order can be changed by dragging and dropping them.

A number of small issues has been fixed and the handling of user roles has been improved.

The help text has been updated to incorporate the new features and to explain the new functionalities.

2. Known issues

If no Kow / Koc have been entered, the following Kps need to be entered to be able to run the assessment: solids-water in soil, solids-water in sediment, solids-water in suspended matter, solids-water in raw sewage sludge in addition to the fractions being directed to sludge, water and air as well as the faction being degraded in the modelled biological sewage treatment plant

Chesar 3.4.1 does not provide the section 3 of the SDS ES for complex substances

2.1. Suggestions to best use Chesar 3.4.1

- Do not set your browser option so that it remembers your password. If you do so, in some cases, you may not be able to connect again as the encrypted password is then saved to your database.
- With some browsers you may be confronted to a slightly different user interface with no effect on the data. If an incorrect user interface is instead displayed, delete the browser history to get it back to normal.
- Our recommendation is to run Chesar 3.4.1 with IUCLID 6.3. If instead you decide to run Chesar 3.4.1 with IUCLID 6.2, be aware that the compatibility between the two applications is broken when the user enters some text in the field "Other description" for PROC 0, PC 0, AC 0 in Chesar and tries to synchronise the uses with IUCLID 6.2. As a workaround, users should temporarily delete the "Other description" texts from Chesar, proceed with the synchronization, add the "Other description" manually to IUCLID and finally retype it to Chesar.
- In order to have a proper transfer of information between Chesar 3.3 and Chesar 3.4.1 we recommend migrating your database from Chesar 3.3 to Chesar 3.4.1, as explained in the Chesar installation manuals (section 5. Upgrade from Chesar 3.0/3.1/3.2/3.3 to Chesar 3.4.1).