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TRISKELION
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report

report no. 11/17

Transcription of Concawe chemical safety assessments into Chesar: summary of a pilot project & current status

ISBN 978-2-87567-077-9

Transcription of Concawe chemical safety assessments into Chesar: summary of a pilot project & current status

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Brussels
November 2017

ABSTRACT

Registration dossiers for petroleum substances (PS) under the European chemicals control legislation REACH require Chemical Safety Assessments (CSAs) as the basis for the identification of operational conditions and risk management measures that ensure safe use.

A pilot study was conducted to assess the suitability of transcribing the Concawe CSAs into Chesar version 2.2. The aim was to identify areas that could affect the effective use of the Chesar tool as a vehicle for developing CSAs for PS with respect to human exposure and, where required, to describe possible methods for handling limitations resulting from the use of the Chesar tool.

In total, 10 significant limitations in the transcription of the petroleum substance CSA into Chesar were identified in this pilot project. For almost all limitations, an acceptable workaround has been identified in the Chesar v2.2 tool. One exception, where no workaround could be found, was a limitation related to the semi-volatile nature of the substance that would allow the use of different Derived No Effect Levels (DNELs) and different exposure assessments for different forms of the substance in one Chesar file. However, since the conclusion of this pilot, most limitations have been addressed in Chesar 3.2 and new functionalities have been added so that workarounds are no longer needed. A functionality to handle semi-volatile substances has also been built in Chesar 3.2.

An important benefit is the efficiency of the Chesar tool functionalities of copying assessments and assessment elements and the Concawe grouping approach. The initial workload of introducing a PS into Chesar is extensive.

In summary, the Chesar tool is suitable to conduct human health CSAs for petroleum substances. The initial workload of introducing such substances can be extensive but once key assessment elements are formed, beneficial functions in Chesar enable useful efficiencies be obtained in updating and managing Concawe dossiers.

KEYWORDS

Chesar tool, chemical safety assessment, exposure assessment, exposure scenario, risk management measures

INTERNET

This report is available as an Adobe pdf file on the Concawe website (www.concawe.org).

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1. INTRODUCTION

Chesar stands for *Chemical Safety Assessment and Reporting*. The tool has been developed by the European Chemicals Agency (ECHA) for supporting registrants under REACH (Registration, Evaluation and Authorisation of Chemicals). All the information related to substance intrinsic properties needed for exposure assessment and risk characterisation are directly imported by Chesar from the endpoint summaries of the respective IUCLID file. Once the assessment has been finalised, the uses reported in Chesar can be exported to IUCLID section 3.5 (Life cycle description) and the Exposure Scenarios, exposure and risk assessment to IUCLID section 3.7 (Exposure Scenarios, exposure and risk assessment). Chesar also facilitates the re-use (or update) of assessment elements generated in Chesar for a single substance to other substances in Chesar.

The approach for creating Chemical Safety Reports (CSRs) adopted by Concawe in 2010 resulted in comprehensive Chemical Safety Assessments (CSAs) for petroleum substances (PS). Until now, CSAs could be simply attached in any form that was convenient for the registrant to the IUCLID file. However, ECHA indicated that the exposure scenario section in IUCLID (section 3.7) will require proper population in the future, which means that CSAs need to be entered in a format that IUCLID can handle in the future. In this respect, the capabilities of Chesar v2.2 to process the information required to develop comprehensive CSAs for PS related to the human exposure were evaluated.

To develop the Exposure Scenarios (ES) for each Use title, it was necessary to map the typical Operational Conditions (OCs) and associated Risk Management Measures (RMMs). Concawe took as a starting point the generic mapping prepared by the solvents sector (European Solvents Industry Group, ESIG) and extended this where Generic Exposure Scenarios (GESs) were inappropriate for PS (as described in Concawe Report 11/12).

The Concawe approach for preparing the human health part of petroleum substances' CSAs is based on the ECETOC Targeted Risk Assessment (TRA) model. The TRA model is developed as a Microsoft Excel application. CSAs can be refined by adding additional modifiers. This approach also allows more flexibility to assess specific exposure situations (e.g. exposure to aerosol mists) and the consideration of RMMs and OCs that are outside the domain of the TRA, which in this report will be called a non-standard approach.

The purpose of this pilot project was to identify and determine the suitability of applying the Chesar v2.2 tool to the petroleum substance CSAs using the Concawe GES and Concawe approach for the preparation of CSA for PS. This was done by carrying out a human health CSA of a representative Concawe substance category in the Chesar tool. The selection of the substance was based on prior experiences when working with the Chesar v2.2 tool and the existing knowledge on the specific CSA within Concawe.

The aim of the pilot project was to identify areas that could impact the effective use of the Chesar tool for PS with respect to human exposure and, where required, to describe possible methods for handling limitations resulting from the use of the Chesar tool.

2. IDENTIFIED TECHNICAL LIMITATIONS OF CHESAR V2.2

The pilot study identified several limitations with Chesar v2.2. This report documents the early constraints preventing effective use of the Chesar tool for PS. Limitations were reported together with suggested approaches for improvement. Early experiences in using the Chesar tool are also included for historical reference.

In this pilot study, a representative Concawe CSA was chosen to be partly converted into Chesar v2.2. Even though the project focused on human health part of the CSA, where elements of environmental or physico-chemical safety assessment interact with the human health CSA in Chesar, these elements are also mentioned.

All fields in Chesar were populated as necessary, i.e. to assure that all different situations which might possibly cause problems and/or require to deviate from the current Concawe approach (cf. Concawe report 11/12), are addressed adequately. A representative selection of contributing ES were identified (Appendix 1) and the respective CSA have been carried out in the Chesar Tool. The selection covered both, the 'standard' approach (i.e. first tier Exposure Assessment using the ECETOC TRA tool) as well as the specific points requiring attention due to the 'non-standard' approach required for addressing the risks presented by some PS (e.g. exposure assessments performed using a modified version of the ECETOC TRA).

In total, 10 significant limitations were identified in the pilot project. For almost all limitations, an acceptable workaround has been identified. This led to an increased work effort and a longer CSR. One significant limitation, with no workaround in Chesar 2.2 was related to the semi-volatile nature of some substances that require the use of different DNELs and different exposure assessments for different forms of the substance within one Chesar file (e.g. the vapour fraction and the aerosol fraction of a substance during spraying activities).

Below is a summary of the most important constraints limiting the effective use of the Chesar tool that were identified during the pilot project and how ECHA has improved the Chesar tool (current version 3.2) with respect to the limitations identified in this report.

Intrinsic properties. All information related to substance intrinsic properties needed for exposure assessment and risk characterisation must be imported by Chesar from the endpoint summaries contained in IUCLID. This has the advantage that consistency between IUCLID and the CSA is automatically ensured.

The following main obstacles limiting the effective use of the Chesar tool for Concawe with respect to this element were identified:

(1) A chemical substance of Unknown or Variable Composition, Complex Reaction Products and Biological Materials (UVCB substance) is not assigned a specific molecular weight, which is required for the ECETOC TRA plugged-in tool in Chesar, but a molecular weight range.

Situation in Chesar v3.2: There is now the possibility to import an upper and lower molecular weight from IUCLID as well as setting a specific molecular weight directly in Chesar, which is then used for the ECETOC TRA assessment.

(2) Semi-volatile substances, such as e.g. heavy petroleum fractions, may require, when dispersed in air, different DNELs for the aerosol and vapour fraction. It is however not possible to assign more than one value for a specific end-point in IUCLID.

Situation in Chesar v3.2: Within one substance several "assessment entities" can be created now. Each assessment entity can be mapped to a separate set of physico-chemical properties and (eco)toxicological endpoints. Thus, it is possible to assess the aerosol and vapour fraction separately in each contributing exposure scenario.

(3) Chesar determines the scope of the human health assessment by the entries in the end-point summary of section 7 of IUCLID (toxicological information). It is not possible to alter the scope to include for example a qualitative assessment for physico-chemical hazards like flammability.

Situation in Chesar v3.2. The scope of assessment still does not take physico-chemical hazards into account. If there are no other qualitative assessments required, it is not possible to justify in the qualitative assessment box the additional modifiers in the Exposure Scenario related to the physico-chemical hazards.

Moreover, Section 3 of the exposure scenario for communication (which reports the methodology that has been applied to develop the exposure estimation) also lacks to mention the qualitative assessment.

(4) In the plugged-in ECETOC TRA tool in Chesar the physical state of the substance cannot be modified.

Situation in Chesar v3.2: The physical state of the substance can be adjusted in each contributing exposure scenario separately.

(5) If required fields related to substance intrinsic properties are not complete or incorrectly entered in IUCLID, extra steps are needed to update IUCLID and re-import the data in Chesar.

Situation in Chesar v3.2: There is now the possibility to edit fields related to intrinsic properties directly in Chesar.

Lifecycle Tree. The Concawe (generic) Exposure Scenarios were, without restructuring, transposed to the Chesar Lifecycle Tree. The following main obstacles limiting the effective use of the Chesar tool for Concawe with respect to this element were identified:

(6) It is generally only possible to assign one Environmental Release Category (ERC) for each identified use. Assignment of ERCs is therefore limited compared to the Concawe CSA.

Situation in Chesar v3.2: There is now the possibility to add as many ERCs as necessary to each identified use.

(7) It is not possible to combine Contributing Scenarios (CSs) in Chesar. This leads to many duplicates within the dossier and thereby to a lengthier CSR.

Situation in Chesar v3.2: There is now the possibility to add as many Process Categories (PROCs) as necessary to each CS. The PROC defined as main PROC is used in the exposure assessment of the respective CS.

Quantitative exposure assessments. Initially 10 'standard' CS assessed with the plugged-in first tier human exposure assessment tool ECETOC TRA v3 were introduced in Chesar and 20 CSs with a 'non-standard' approach (i.e. exposure assessments performed with a modified version of ECETOC TRA and the ESIG consumer tool) were introduced as inputs from an external exposure tool in Chesar.

The following main obstacle limiting the effective use of the Chesar tool for Concawe with respect to this element was identified:

(8) Introducing all use conditions for the 'non-standard' assessment would be less time-consuming when the order of the determinants could be changed after they have been introduced.

Situation in Chesar v3.2: The position of determinants in the conditions of use list can easily be changed via "drag and drop".

(9) 'Non-standard' conditions of use (i.e. RMMs not covered by ECETOC TRA) can be created in Chesar, but their reduction factors are not considered in the exposure estimates created within Chesar using the built-in ECETOC TRA tool. These reduction factors need to be considered manually outside Chesar at the moment.

Situation in Chesar v3.2: This issue still exists. ECHA is currently in a dialogue with ECETOC to address it in the next versions of Chesar.

Supporting text elements. Various supporting text elements were included in Chesar. These are pieces of text that can be typed or copied into text fields to explain situations or assessments. Most are intended to demonstrate the possibility of providing more information and the supporting text elements should not be viewed as complete and final. Examples of the supporting text elements are e.g. given for some PROCs in 'Conclusion on risk characterisation', e.g. "A quantitative assessment of short term exposure has not been undertaken as there is a difference of at least a factor of 30 between the short term (when expressed over 15 minutes) and the long term DNEL (when expressed over 8 hours) DNELs" and they are given in the field for 'Risk characterisation (qualitative/semi-quantitative)', e.g. "The substance has been classified as carcinogen. When the OCs and RMMs as described in this CS are implemented, the substance will not pose a risk to human health for workers". Such text elements were only included for a few CSs to illustrate the options. The following main obstacle limiting the effective use of the Chesar tool for Concawe with respect to this element was identified:

(10) The comments on assessment approaches are limited to 4000 characters.

Situation in Chesar v3.2: There is no longer a limitation on the character number.

Finalisation from Chesar to CSR in Word format. Finally, Chapters 9-10 of the CSR have been generated by Chesar in RTF format (Rich text format). An export was made of the Chesar file for inclusion into IUCLID (.zip) and an export was made of the Chesar file for sharing with other parties (.chr). In IUCLID, the report generator was used to complete section 3.5 and 3.7 of IUCLID and to generate the full CSR in RTF format (Chapters 1-10). No obstacles limiting the effective use of the Chesar tool for Concawe with respect to this element were identified.

3. DISCUSSION AND CONCLUSIONS

The aim of this project was to identify areas that could impact the effective use of the Chesar tool for PS with respect to human exposure and, where relevant, to describe possible methods for handling limitations resulting from the use of the Chesar tool (workarounds). In total, 10 significant limitations were identified. For most of the limitations resulting from the use of the Chesar tool, a workaround has been found. The length of the CSR prepared using Chesar can lead to a longer Section 9; however, this is off set by the discontinuation of several pages of CSA appendices previously included in Concawe dossiers. .

The pilot substance, for which Chesar was partially completed, contains one ES (use as fuel) with four separate CSs for consumers. These were completed in Chesar. In our test, no specific issues were noted that are only related to consumer assessment in Chesar. The issues that limit the effective and efficient use of Chesar in relation to consumer assessments are not different from those in relation to worker assessment. The main issue was the fact that the exposure assessment tool for consumer exposure (ESIG tool) is an external tool, for which some determinants and the exposure estimates need to be entered manually into Chesar.

Situation in Chesar v3.2: The limitations identified in this report have mostly been solved in the current version of the Chesar tool or will be addressed in the near future. Sole exception is the qualitative safety assessment. The qualitative assessment still does not address physical-chemical hazards and there is a lack of transparency in section 3 of the ES for communication with respect to the qualitative assessment. As far as we know, there are currently no plans by ECHA to improve this situation. In addition, some exposure estimate tools, such as EGRET and ConsExpo, are currently improved to allow the electronic transfer of data between Chesar and these external tools.

An additional advantage of using Chesar is the fact that it acts as a database in which the most recent file is always the starting point for further work. This can be very important when modifications to a CSR are needed, e.g. due to new hazard data or new uses.

Based on the observations discussed in these report, it can be concluded that the Chesar tool is suitable for application for the PS CSAs (human exposure) using the Concawe GES approach. An important factor in this favour is the efficiency of the Chesar tool functionalities of copying assessments and assessment elements and the Concawe grouping approach.

4. GLOSSARY

Acronym	Definition
Chesar	Chemical Safety Assessment and Reporting
CS	Contributing Scenario
CSA	Chemical Safety Assessment
CSR	Chemical Safety Report
DNEL	Derived No Effect Level
ECETOC	European Centre for Ecotoxicology and Toxicology of Chemicals
ECHA	European Chemicals Agency
ERC	Environmental Release Categories
ES	Exposure Scenario
ESIG	European Solvents Industry Group
GES	Generic Exposure Scenario
OC	Operational Condition
PROC	Process Categories
PS	Petroleum Substances
REACH	Registration, Evaluation and Authorisation of CHemicals
RMM	Risk Management Measures
RTF	Rich Text Format
TRA	Targeted Risk Assessment
UVCB	Unknown or Variable Composition, Complex Reaction Products and Biological Materials

5. REFERENCES

1. CONCAWE (2012) Developing human health exposure scenarios for petroleum substances under REACH. Report No. 11/12. Brussels: CONCAWE

APPENDIX 1 - PROPOSAL FOR SELECTION OF THE CONTRIBUTING SCENARIOS AND INFORMATION TO BE INCLUDED IN THE PILOT CHESAR ASSESSMENT

As described in the proposal, the first step of the project was the selection of Contributing Scenarios (CS) used in the Chesar pilot.
The information received from Concawe was investigated in order to make a representative selection to cover:
- 10 'standard' CSs with a first-tier human exposure assessment, performed with ECETOC TRA
- 20 CSs with a 'non-standard' approach, i.e. for which an object must be created in the Chesar RMM library.

For the following **10 'standard' CSs** the Chesar default plugged-in tool ECETOC TRA v3 (TIER1) was used; these 10 CS[1] were selected based on the different PROCs:

1) CS6 - PROC9
2) CS15 - PROC1
3) CS15 - PROC2
4) CS15 - PROC3
5) CS16 - PROC4
6) CS36 - PROC15
7) CS45 - PROC5
8) CS501 -PROC8b
9) CS100 -PROC14
10) CS112/CS10- PROC7

The following **20 CSs with a 'non-standard' approach** were selected to be included in Chesar as external exposure tool estimate:

1) CS3 - PROC8a *[1]*
2) CS5 - PROC8a [*1]*
3) CS34 + CS22 - PROC8a *[1]*
4) CS3, CS8, CS22 - PROC9 *[1]*
5) CS95 - PROC4 *[2]*
6) CS16 - PROC4 *[2]*
7) CS97 - PROC7 *[2]*
8) CS44 - PROC7 *[2]*
9) CS136 - PROC3 *[3]*
10) CS77 - PROC8b *[3]*
11) CS24 - PROC7 *[3]*
12) CS32,CS108 - PROC6 *[3]*
13) CS10,CS34, CS109 - PROC11 *[3]*
14) CS44, CS10, OC8 - PROC11 *[4]*
15) CS34, CS48, CS47, CS50, CS51 - PROC10 *[4]*
16-20) Consumer uses in liquid fuel *[5]*

The Concawe's comprehensive CSAs contain various 'non-standard' approaches which may be briefly categorised as following:

- [1] The worker CSA contains **additional exposure modifiers** (besides the default ECETOC TRA modifiers), related to **specific risk management measures** such as the

[1] Encoding of the CS based on Concawe document '*20120408 SRGOs cm rev0_JU_5June2012draft revAM 11-06-2012*'

use of drum pumps and the measures to 'Drain down system prior to equipment break-in or maintenance' *[see CS 1-4 above].*

- [2] The worker CSA contains **additional exposure modifiers** (besides the default ECETOC TRA modifiers), related to **common operational conditions** like the use of good general ventilation or the partial enclosure of a high-pressure washer *[see CS 5-8 above].*

- [3] The worker CSA contains an **initial estimated exposure modification from ECETOC TRA** based on the nature of the Concawe processes and substances, such as the elevated temperature of some processes and the semi-volatile nature of the substances which requires that in addition to aerosol exposures for selected PROCs vapour exposures were included *[see CS 9-13 above].*

- [4] The worker CSA contains **additional exposure modifiers** (besides the default ECETOC TRA modifiers), due to **specific risk management measures related to the product properties** (concentration in the product) *[see CS 14-15 above].*

- [5] The **Consumer exposure** was estimated with a tool which is not a plugin of Chesar, so for all determinants an object will have to be created in the Chesar library *[see CS 16-20 above].*

CSs were selected so that all 'non-standard' approaches contained in the CSA of Concawe will be in equal extent part of this pilot project. A specific type of 'non-standard' approach was included twice so that it is possible to evaluate the efficiency of using objects already contained in the library.

Furthermore the following tasks were carried out:

- include a **qualitative CSA approach** for CARCINOGENIC HAZARD (R45/H350) plus relevant additional determinants from the library for:
  1) CS15 - PROC1
  2) CS15 - PROC2
  3) CS15 - PROC3
  4) CS36 - PROC15
  5) CS501 - PROC8b
- include supportive information on **actual measurement** data with reference to the original source;
- **copy** the created CSs **to other Exposure Scenarios** thereby creating a more complete CSA;
- include the steps to **generate a CSR.**

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