LCID Methodology Guide Update and Preliminary Test Results

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Cefic/VCI Mixtures Task Force
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LCID team

LCID sub-team created:

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- Christian Bögi, BASF
- Marc Brulport, Merck
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- Donna Seid, Ashland
- Stefanie Welz, BASF
Agenda

1. Background of Cefic/VCI project on mixtures
2. Test run of LCID methodology
3. Preliminary results
4. Next steps
Safe use information for mixtures

1. Chemical mixture
   - CLP Screening 1: Is mixture classified as hazardous?
     - Yes: CLP Screening 2: Identify H&P phrases
     - No: No specific approach is required. Document

2. Consider sector “Bottom-up” approach
   - Is there an industry sector “Bottom-up” approach that is applicable?
     - Yes
     - No: Apply Cefic/VCI “Top-down” approach (LCID methodology)
If the risks are controlled for the most hazardous component, then the risks from the other substances in the mixture are also likely controlled.
LCID methodology (high level)

1. Compile Exposure Scenarios of Components
2. Identify components which drive CLP hazard classifications of mixture
3. Identify Priority Substances, and Lead Components, local effects per exposure route/pathway
4. Consolidate OCs and RMMs based on identifications
5. Embed in SDS
6. Append to SDS
Background

Presented several approaches being developed

ENES 4

Interim reporting on LCID methodology

ENES 5

Presented draft LCID methodology

ENES 6

Presented preliminary outcome consultation

ENES 7

Test run LCID methodology Aug./Sept. 2015

ENES 8

Prelim. results of test run

ENES 9

2013

2014

2015

• Mapping available approaches to generate safe use info for mixtures
  • 2 main approaches
    • Generally applicable (top down)
    • Sector-specific (bottom up)

• Development of common concept for a top down methodology
  LCID methodology

• Both approaches are complementary to each other

• Bottom up approaches are further developed by sector associations - working together to:
  • Exchange experiences
  • Find harmonised solutions for similar challenges
  • Align as much as possible sector-specific methodologies
  • Agree on terminology

Action 4.4.A

Publication of Practical Guide & Tool

Action 4.4.B
Comments on LCID guide and tool

**Received**
- 12 contributions
- > 140 comments by Feb. 2015
  - Nordic working group comments

**Reviewed**
- Filtered (e.g., by content, clarification, Guide/Tool)
- Grouped like comments
- Incorporated changes, as appropriate

**Responded**
- Delivered responses to commenters by the beginning of November 2015
Agenda

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Testing comprehension of LCID methodology

- **Objective:**
  - Is outcome of the LCID methodology reproducible, independent of user?
  - Is the LCID Guide and tool sufficiently elaborated to enable the user to apply the methodology in an appropriate way?

- **How?**
  - Different people apply the LCID methodology independent of each other for the same examples.
Examples

- Realistic formulations as possible
- Demonstrate understanding of various scenarios:
  - Priority Substances present
  - DNELs available
  - Back-up approach
  - Groupings
  - Case-by-case basis
## Templates for manual calculations

### Table: Description of Data Fields

<table>
<thead>
<tr>
<th>Data Element</th>
<th>Description</th>
<th>Contribution/Use</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Name of Exposure Scenario/Contributing Scenario</td>
<td>Name of Exposure Scenario/Contributing Scenario</td>
<td>Fields to be completed by Test Panel</td>
<td>Name of Exposure Scenario/Contributing Scenario</td>
</tr>
<tr>
<td>Derived Safe Use Information</td>
<td>Derived safe use information</td>
<td>Fields pre-populated for mixture</td>
<td>Derived safe use information</td>
</tr>
</tbody>
</table>

### Example Table

<table>
<thead>
<tr>
<th>Value</th>
<th>Description</th>
<th>Contribution/Use</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>12.34</td>
<td>Parameter A</td>
<td>Test Panel</td>
<td>Additional notes</td>
</tr>
<tr>
<td>5.67</td>
<td>Parameter B</td>
<td>Test Panel</td>
<td>Additional notes</td>
</tr>
</tbody>
</table>

### Diagram: Example Diagram

- **Fields pre-populated for mixture**
- **Fields to be completed by Test Panel**
- **Name of Exposure Scenario/Contributing Scenario**
- **Derived safe use information**
Templates for LCID tool calculations

Short Instruction on how to use the LCID template

- mandatory inputs
- optional inputs
- conditional inputs
Instruction form

[Text Run of LCID Methodology: Instructions and Evaluation Form]

Introduction
Thank you for your interest in participating in this top-run of applying the LCID methodology to complete the dataset. Please familiarize yourself with the underlying principles and structure of the LCID methodology as documented in detail in Chapter 7 of the 'Smart Reach Practical Guide on Exposure Assessment and Harmonisation in the REACH REGULATIONS' document. You can find this information online at: [link to the document].

At the beginning of this document, you will find instructions on how to perform the LCID methodology. You are requested to identify the source of information for features provided in the attached spreadsheet. If this information is not available in the spreadsheet, you are expected to fill in the data fields and formulate to gather further information, and 1 data file is saved using the naming convention.

The data provided for each molecule is complete and contains all the necessary data to apply the LCID methodology. Make sure that no other data is added or modified.

In order to ensure a correct and complete dataset, the pre-screened data may not be changed after completing the evaluation phase.

Each spreadsheet also contains a list of empty fields (a list of fields that are not used in the LCID methodology). These empty fields must be completed by the user to document the final result and to facilitate (e.g., for hazard calculations).

You are only required to complete those fields that contain valuable information, and you are expected to fill in the data fields.

The completed worksheet should be returned by 20 September 2013.

If you have any questions or need further assistance, please feel free to contact us at [contact information].

We are conducting an Excel-based LCID tool that has been designed to support users in identifying the Local Compounds for the relevant exposure assessment and pathways. By entering the pre-screened data, you will receive instruction on the most relevant and associated reference values (e.g., CEC, PREDICT, etc.). The information is presented in a clear and easy-to-follow format. It is important to note that this information is not intended to replace the final decision and that you should still conduct your own review and evaluation regarding the appropriateness of the LCID methodology.

If you have any questions or need further assistance, please feel free to contact us at [contact information].

In addition to the information provided in this document, we are seeking to complete the following tasks:

- Description of templates
- No need to gather further information
- Save spreadsheets using a given naming convention
Evaluation form

• Identification information

• Able to run the methodology manually? using the tool?

• Able to derive Lead Components?

• Feedback on instructions, example results, manual/tool calculations
Delivered on 25 August 2015

1. Updated Practical Guide and LCID Tool with examples
2. Test examples with templates
3. Deadline for response
4. Volunteers representing industry, consultants, Competent Authorities, ECHA

Deadline: 25.9.15
1. Background of Cefic/VCI project on mixtures
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Respondents

27
- Total
- 12 manufacturers, importers, downstream users, distributors
- 6 consultants
- 7 authorities
- 1 software supplier
- 1 N/A

12
- Did all examples
- 13 partial
- 2 N/A

5
- Calculated manually and with tool
- 7 manually only
- 2 used tool only
- 11 partial tool/manual
- 2 N/A

Main reason for not completing—time constraints
“We really like this whole study and approach. Congratulations! It’s very helpful and I hope I can work further to have this implemented in our IT system. It’s the best approach (for us) from several others that we have ‘evaluated ‘ until now.”

“…powerful tool, more clear arrangement of the end result wishful…”

“…the guidance and the tool provided for the most part make intuitive sense and meet the intended purpose. The biggest problem in applying this guidance is the vast increase in complexity and technicality…”

“LCID tool is a good tool for assistance, especially in proofing the results of calculations. However, it does not substitute expert judgment.”

“…workshop would be preferable…”
General comments: summary

- Both guidance and tool are comprehensive and easy to use
- Application of the methodology is challenging if needed for a large number of mixtures
- Ease of use and results strongly depend on data availability
- Expert judgment is still necessary
- Need for further IT support of the calculation tool or the separate development of software solutions
- Training workshops would be appreciated

No show stoppers!
Human health: preliminary results

Test run was successful

- LCID methodology was generally well understood
- Able to identify underlying principles
- Calculation tool delivered reliable results
- Method proved to be robust
- Valuable comments were received for a refinement of the examples and further improvements
Reasons for differences when compared to results from LCID group

- Minor mistakes, e.g., mathematical errors
- (Mis)identification of relevant components
- Template was not correctly completed
- (Mis)groupings (e.g., selection of two inhalation lead components)
- A case-by-case assessment was missed
- Not all data needed was entered correctly in tool, e.g., DNELs
Environment
Environment: preliminary results

- Examples received in total
- Identified Lead Component
- Derived safe use information for mixtures
Topics

• Identification of Lead Component (LC) (both PNEC- and backup/classification approach)
• Ozone hazard
• Priority Substance (e.g., PBT)
• Mixture not classified for environmental hazards
• $M_{\text{safe}}$ for mixture (calculation of modifying factor, $C_{\text{weighted}}$)
• OCs / RMMs for mixture
Lead Component Identification

12% Failure
Testers did:
• mix up PNEC- and backup approach
• not spot PBT compound and failed to identify LC due to missing data
• claim missing info for non-classified components

88% Correct answer
Testers did:
• identify correct LC (via PNEC- or backup approach, also for ozone hazards)
• spot PBT component
• stop the procedure because of the classification of the mixture
$M_{\text{safe}}$, OCs/RMMs

19% Failure

Testers did:
- correctly calculate the modifying factor and $C_{\text{weighted}}$ correctly, but used concentration of LC to derive $M_{\text{safe}}$
- not consider grouping components

49% Correct answer

Testers did:
- correctly calculate the modifying factor, $C_{\text{weighted}}$ and $M_{\text{safe}}$ (for the mixture)
- derived appropriate OCs and RMMs for the product

49 + 32* = 81%

*division by XY% instead of 0.XY
Environment: preliminary results

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1. **Background of Cefic/VCI project on mixtures**
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4. **Next steps**
Next steps

- Finalize assessment of test results
- Update Practical Guide by Q4 2015
- Update LCID Tool by Q4 2015
- Define and commence execution on communication plan
- Involve IT providers in LCID methodology launch
- Workshop in 2016
Questions