Retrofit Design of Generic Exposure Scenarios for Substances in Complex Mixtures

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Exposure Assessment by Formulator for Substances in Mixtures

Industrial and professional users	Safety data sheet	Exposure assessment	Implementation at company level
Mixture non hazardous, no substance above declaration threshold	Voluntary	Voluntary	No RCR calculation, no scaling option; Good practice advice
Mixture non hazardous, one or more substance above declaration threshold 1% < Conc(Xn) < 25 %* 1% < Conc(Xi) < 20 % / 10 %	On request	Mandatory according to REACH article 14	Exposure assessment related to hazard characteristics
Mixture hazardous 25 % < Conc(Xn)* 20 % / 10 % < Conc(Xi)	Mandatory	Mandatory	Exposure assessment related to hazard characteristics

* Default concentration figures, may be different for specific substances, further hazards to be considered

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Basic Considerations

- REACH does not require assessment of mixtures as such

However :

- REACH demands assessment of hazardous substances in mixtures
- REACH demands communication of assessment results
- Communication may be required even if SDS is not mandatory (in line with REACH article 32)
- Formulators as well as end-users have to ensure compliance with regard to conditions for safe use

ES Communication Downstream 1

- Precondition : Sufficient information about raw materials is available

✓ REACH information available for more than 90 % of compositions (solvents/amines/reactive diluants registered 2010, polymers/natural oils and minerals exempt, pigments/extenders/water non hazardous)

- Proposal A : **Create clusters of similar mixtures and derive homogeneous conditions of use from compositional information**

✓ Viable for relatively simple mixtures, e.g. putties, wall paints

✓ May need information exchange between different manufacturers

❖ Not viable for complex product portfolios of a company with e.g.

– More than 60,000 active formulas, more than 4,000 raw materials

– More than 200 lead substances (DPD+) or 10 clusters for powders

ES Communication Downstream 2

- Proposal B : **Consolidated exposure assessment for substances**
- Mixture may contain 10 disclosed substances with 20 relevant risks
- Per substance 8 DNELs (worker) and 8 PNECs may be provided
- Different assessment tools used, especially for environment

✓ Consolidation is viable (example from DuPont Performance Coatings)
- when parameters are focused (longterm systemic, surface water)
- when lead/priority substances are identified
- when integrative assessment tool can be used (ECETOC, spERCs)
- when expert judgment is accepted (solids in liquids, spray, reactants)
- when scaling with regard to substance concentration is accepted

➢ Calculation of individual RCR/M(safe) values for 20 sets of OCs/RMMs

❖ Display of results in an annex is disliked by recipients‘ associations

Expectations from End-user Business Associations

- Proposal ACEA and other industrial/professional end-users‘ business associations
- Clear text description of standard use conditions in the sector (one set of paramaters for all comparable products from all suppliers)
- Indication of safe use (RCR < 1)
- Limitation of communication to core data and risk management measures (according to REACH article 14 (6) and article 31 (7))
- Integration into core SDS (e.g. into section 8.2/8.3)
- Scaling via internet link if necessary

ES Communication Downstream 3

- Proposal C : **Create defined sets of standard OCs/RMMs for different of application and derive tolerable DNELs/PNECs**
  - Standard sets for [setting + PROC + LEV/TRV + RMM] can be defined for DOA > 4 h
  - Starting from requirement „safe use“ (RCR ≤ 1), inverse calculation according to ECETOC TRA version 3 leads to a set of tolerable DNELs (similar to M(safe) derivation for environmental assessment)
  - Raw materials can be compared versus tolerable DNELs
  - ➢ Communication only confirms „safe use“ for standard conditions

- Additional considerations
- Condense received information to essential needs
- Apply approved spERC concepts from downstream user associations
- Translate abstract use descriptors to sector specific language

Refinish Bodyshop as Practical Example

- Refinish bodyshop uses about 300 products from multiple suppliers
- Different use patterns are considered for waterborne spray coatings, solventborne spray coatings, putties applied with a knife, activators for spray coatings, activators for putties, thinners, degreasers and cleaning solvents
- Users mix > 10,000 colour shades, add hardener, adjust viscosity
- Professional use in a close-to-industrial setting
- Environmental assessment for point sources (AIRC spERCs)
- All products are used under similar operational conditions
- Users will probably not vary OCs and RMMs from product to product
- Users are far away from being experts for safety assessment and are probably not able to apply scaling or to use similar tools
- ➢ Basic assessment of typical OCs and RMMs provided by CEPE

CEPE Use Mapping with OCs and RMMs

Preparing, transferring/loading, application by spraying, drying and curing of coating material					
	PROC	DOA	LEV/TRV	RPE	DPE
Mixing	5 (covering 3)	> 4 h	TRV 5-10 ac/h	no	yes level 2
Transferring	8a (covering 8b)	> 4 h	TRV 5-10 ac/h	no	yes level 2
Non-industrial spraying	11	> 4 h	LEV equivalent	yes due to aerosol	yes level 2
Curing	4 (covering 2)	> 4 h	TRV 5-10 ac/h	no	yes level 2

Preparing, transferring/loading, application with a putty knife, drying and curing of putty					
	PROC	DOA	LEV/TRV	RPE	DPE
Mixing	5 (covering 3)	> 4 h	TRV 5-10 ac/h	no	yes level 2
Transferring	8a (covering 8b)	> 4 h	TRV 5-10 ac/h	no	yes level 2
Applying with putty knife	10	> 4 h	TRV 5-10 ac/h	no	yes level 2
Curing	4 (covering 2)	> 4 h	TRV 5-10 ac/h	no	yes level 2

Sanding of cured coating					
	PROC	DOA	LEV/TRV	RPE	DPE
Sanding	24	> 4 h	LEV	no	yes level 2

Inverse Calculation of Tolerable DNELs

PROC	Fugacity	Ventilation	DOA	RPE	DPE	Content range of lead substance (Inhalative)*				Content range of lead substance (Dermal)*			
		Indoor				> 25 %	> 5 - 25 %	> 1 - 5 %	< = 1 %	> 25 %	> 5 - 25 %	> 1 - 5 %	< = 1 %
4	Liquid low	TRV	> 4 - 8 h	no	no	3 ppm	1,8	0,6	0,3	**6,86 mg/kg**	4,12	1,37	0,69
4	Liquid med	TRV	> 4 - 8 h	no	no	15 ppm	9	3	1,5	**6,86 mg/kg**	4,12	1,37	0,69
4	Liquid high	TRV	> 4 - 8 h	no	no	75 ppm	45	15	7,5	6,86 mg/kg	4,12	1,37	0,69
4	Solid low	TRV	> 4 - 8 h	no	no	0,3 mg/m³	0,18	0,06	0,03	6,86 mg/kg	4,12	1,37	0,69
5	Liquid low	TRV	> 4 - 8 h	no	yes	3 ppm	1,8	0,6	0,3	1,37 mg/kg	0,82	0,27	0,14
5	Liquid med	TRV	> 4 - 8 h	no	yes	**30 ppm**	18	6	3	1,37 mg/kg	0,82	0,27	0,14
5	Liquid high	TRV	> 4 - 8 h	no	yes	150 ppm	90	30	15	1,37 mg/kg	0,82	0,27	0,14
5	Solid low	TRV	> 4 - 8 h	no	yes	0,3 mg/m³	0,18	0,06	0,03	1,37 mg/kg	0,82	0,27	0,14
8a	Liquid low	TRV	> 4 - 8 h	no	yes	**7,5 ppm**	4,5	1,5	0,75	1,37 mg/kg	0,82	0,27	0,14
8a	Liquid med	TRV	> 4 - 8 h	no	yes	**30 ppm**	18	6	3	1,37 mg/kg	0,82	0,27	0,14
8a	Liquid high	TRV	> 4 - 8 h	no	yes	150 ppm	90	30	15	1,37 mg/kg	0,82	0,27	0,14
8a	Solid low	TRV	> 4 - 8 h	no	yes	0,15 mg/m³	0,09	0,03	0,015	1,37 mg/kg	0,82	0,27	0,14
10	Liquid low	TRV	> 4 - 8 h	no	yes	**7,5 ppm**	4,5	1,5	0,75	2,74 mg/kg	1,65	0,55	0,27
10	Liquid med	TRV	> 4 - 8 h	no	yes	**30 ppm**	18	6	3	2,74 mg/kg	1,65	0,55	0,27
10	Liquid high	TRV	> 4 - 8 h	no	yes	150 ppm	90	30	15	2,74 mg/kg	1,65	0,55	0,27
10	Solid low	TRV	> 4 - 8 h	no	yes	0,15 mg/m³	0,09	0,03	0,015	2,74 mg/kg	1,65	0,55	0,27
11	Liquid low	LEV	> 4 - 8 h	yes	yes	2 ppm	1,2	0,4	0,2	2,14 mg/kg	1,29	0,43	0,21
11	Liquid med	LEV	> 4 - 8 h	yes	yes	10 ppm	6	2	1	2,14 mg/kg	1,29	0,43	0,21
11	Liquid high	LEV	> 4 - 8 h	yes	yes	20 ppm	12	4	2	2,14 mg/kg	1,29	0,43	0,21
11	Solid high	LEV	> 4 - 8 h	yes	yes	4 mg/m³	2,4	0,8	0,4	2,14 mg/kg	1,29	0,43	0,21
24	Solid high	LEV	> 4 - 8 h	yes	yes	0,5 mg/m³	0,3	0,1	0,05	0,71 mg/kg	0,43	0,14	0,07

Issues Around Critical DNELs 1

- **> 30 ppm (medium vol.)/7.5 ppm (low vol.)/6.86 mg/kg.d**
  - All substances with higher DNELs lead to RCR < 1 for professional use under confined conditions
  - No issues with cumulation rule as this threshold applies for > 25 % substance content in a mixture
  - No issues known for combined effects (RCR inhalative + RCR dermal, e.g. n-butanol, butoxyethanol, cyclohexane ,toluene)

- **30 ppm** **Hydrocarbons** (UVCBs, DNEL inhalative 150 mg/m³)
  - ppm value depends on molecular mass (120 g or 125 g)
  - No dermal risk phrase/hazard statement assigned
  - No cumulation issue as exposure estimate covers up to 100 %
  - Borderline case for professional use

Issues Around Critical DNELs 2

- **20 ppm** **Styrene**
  - Release below 10 % from spray putties with 32 % content and below 3 % from putties for application with knife with 16 % content
  - DNEL dermal relatively high, no issue with combined impact

- **20 ppm** **Methyisoamylketone, Methylisobutylketone**
  - Restrictions of DOA or LEV or RPE if concentration > 25 %
  - Reassessment of cumulation rule if concentration < 25 %

- **17.5 ppm** **Technical xylene** (multiconstituent substance or UVCB)
  - DNEL refers to ethyl benzene (15 - 25 % content), xylene is 50 ppm
  - Discussions with suppliers how to avoid unreasonable restrictions

Issues Around Critical DNELs 3

- **2 ppm Amines**
- Limited content in finished products (< 1 % or 1 - 5 %)
- Reassessment of cumulation rule may be necessary

- **2 ppm / 1.23 mg/kg.d Phenol**
- Limited content in products (< 1 %) or separate set of OCs / RMMs

- **0.8 ppm Kresol**
- Replacement of major part by phenol in wire enamels

- **0.006 mg/m³Lead Chromate**
- No safe use derived from calculations; complete phase-out

How to Communicate Results of Exposure Assessment ?

- More than 90 % of information from received ESs fit into standard frames for OCs and RMMs (Option C)
- Standardization of use patterns is also suitable for provided information which does not disclose 100 % composition of mixtures
- Less than 10 % of information from received ESs lead to unusual restrictions (DOA < 4h, LEV instead of TRV, unusual PPE) and may trigger more complex exposure communication (Option B)
- ❖ Imported substances and DU chemical safety assessment may trigger need for an annexed exposure assessment
- ❖ EChA or Member states competent authorities may consider consolidation activities by formulators as DU CSA rather than scaling which would enlarge communication requirements
- ❖ Also simplified communication needs complex assessment and documentation in its background

How Simple Communication May Look Like

All raw materials for this formulation are (pre)registered under REACH and cover following activities:					
Preparing, transferring/loading, application by spraying, drying and curing of coating material					
	PROC	DOA	LEV/TRV	RPE	DPE
Mixing	5 (covering 3)	> 4 h	TRV 5-10 ac/h	no	yes level 2
Transferring	8a (covering 8b)	> 4 h	TRV 5-10 ac/h	no	yes level 2
Non-industrial spraying	11	> 4 h	LEV equivalent	yes due to aerosol	yes level 2
Curing	4 (covering 2)	> 4 h	TRV 5-10 ac/h	no	yes level 2
Use of the mixture is considered safe when conditions for safe use of the lead or priority substances are respected (all risk characterization ratios below 1).					
This formulation does not contain substances with identified hazards which may require untypical conditions of use and unusual risk management measures.					
The additional assessment beyond REACH (residual monomer content, impurities) does not lead to diverging conclusions.					
Exposure assessment is performed for coating material as supplied. Assessment may require adaptation to ready for use mixture (review hardener and/or diluant). However, no diverging conclusions are expected as long as state of the art hardeners and diluants are added.					
Exposure assessment is performed for application of coating material at ambient temperature. Adaptation may be required for application at elevated temperature (e.g. hot spraying).					
By variation of operational conditions and risk management measures (scaling), a downstream user can check whether he works inside the exposure scenario boundaries. In case of a need for scaling, a downstream user may refer to ……					