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# CONSOLIDATION OF INFORMATION FOR MIXTURES UNDER REACH

## ANALYSIS OF THE DPD<sup>+</sup>-APPROACH

FINAL REPORT – PART I  
ANALYSIS REPORT

Januar, 2012

ENTWURF!



For labels: For: Ökopol GmbH

**Ökopol GmbH**  
**Institut für Ökologie und Politik**  
Nernstweg 32-34  
D-22765 Hamburg

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**ÖKOPOL GmbH**  
**Institut für Ökologie und Politik**

Nernstweg 32–34  
D – 22765 Hamburg  
☎049-40-39 100 2 0  
fax:0049-40-39 100 2 33

[www.oekopol.de](http://www.oekopol.de)

[info@oekopol.de](mailto:info@oekopol.de)

Authors: Antonia Reihlen, Dirk Jepsen, Olaf Wirth

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## Abbreviations

|          |   |
|----------|---|
| ATP      | Adaptation to Technical Progress  |
| BCF      | Bioconcentration Factor   |
| C        | Concentration   |
| CA       | Concentration Addition  |
| Cat      | Category  |
| CC       | Critical Component  |
| CCA      | Critical Component Approach   |
| CLP-Reg. | Classification and Labelling Regulation   |
| C&L      | Classification and Labelling  |
| CEFIC    | European Chemical Industry Council  |
| CSA      | Chemical Safety Assessment  |
| CMR      | Carcinogenic, Mutagenic and Reprotoxic  |
| Conc.    | Concentration (used only in the context of DPD+)                                |
| CoU      | conditions of use (OCs + RMMs)  |
| CSR      | Chemical Safety Report  |
| DPD      | Dangerous Preparation Directive   |
| DSD      | Dangerous Substances Directive  |
| DU       | Downstream User   |
| DU CSR   | Downstream User Chemical Safety Report  |
| EC       | Effect Concentration  |
| ECHA     | European Chemicals Agency   |
| EFSA     | European Food Safety Authority  |
| EINECS   | European Inventory of Existing Chemical Substances                              |
| EPM      | Equilibrium Partitioning Method   |
| eSDS     | Extended Safety Data Sheet  |
| ES       | Exposure Scenario   |
| ESIG     | European Solvent Industry Group   |
| ESR      | Existing Substances Regulation  |
| EU – TGD | European Union Technical Guidance Document on the Risk Assessment of Substances |
| Ex-ECB   | Former European Chemicals Bureau  |
| FEICA    | Association of European Adhesives and Sealants Manufacturers                    |
| IA       | Independent action  |
| IC       | Inhibition Concentration  |
| IPCS     | International Programme for Chemical Safety                                     |
| LC       | Lethal Concentration  |
| LD       | Lethal Dose   |
| LS       | Lead Substance  |
| LSI      | Lead Substance Indicator  |
| MCS      | Multi Constituent Substance   |
| MS       | Member State  |
| NOEC     | No-Effect Concentration   |
| OCs      | operational conditions of use   |
| OECD     | Organization for Economic Co-operation and Development                          |
| OEL      | Occupational Exposure Limit Value   |
| PBT      | Persistent, Bioaccumulative and Toxic Substance                                 |

|      |   |
|------|---|
| PC   | Physico-Chemical  |
| PEC  | Predicted Environmental Concentration   |
| PNEC | Predicted No – Effect Concentration   |
| RAR  | Risk Assessment Report  |
| RCR  | Risk Characterization Ratio   |
| RF   | Release Factor  |
| RMMs | Risk Management Measures  |
| SDS  | Safety Data Sheet   |
| STP  | Sewage Treatment Plant  |
| SVHC | Substance of Very High Concern  |
| TEF  | Toxicity Equivalent Factor  |
| TIE  | Toxicity Identification Evaluation  |
| TNsG | Technical Notes for Guidance  |
| TU   | Toxic Unit  |
| UBA  | Umweltbundesamt (German Federal Environment Agency)   |
| UVCB | Substances of Unknown or Variable Composition, Complex Reaction Products and Biological Materials |
| vPvB | very Persistent and very Bioaccumulative Substance  |

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# 1 INTRODUCTION

## 1.1 Context

The identification and communication of safe conditions of use (CoU) including risk management measures (RMM) for substances is one central mechanism of REACH to improve the level of protection of human health and the environment.

Formulators play a crucial role in the communication along the chemicals supply chains: they ensure a proper link between substance registrants and end-users of substances as such, in mixtures or in articles. Formulators frequently have a good understanding of the chemistry of substances and mixtures as well as the conditions under which they are applied by their end-users. They are required to forward received information to their customers in an “adequate form”; i.e. a form that is understandable and helpful and takes account of all the substances eventually present in a mixture.

The core questions analysed in this project were how two tasks of formulators can be efficiently performed. These are:

- Task 1– Identification of operational conditions (OCs) and RMMs ensuring safe use of all substances and mixtures contained in a produced mixture, based on the information received from substance and mixtures suppliers<sup>1</sup> or generated by himself<sup>2</sup> - and
- Task 2 – Processing and forwarding that information in an understandable language and manageable form to the customers.

These two tasks are commonly called “consolidation of information”. The term “consolidation” does not exist in the REACH text but evolved in the discussion on the downstream user (DU) obligations during REACH implementation..

The consolidation process is not entirely new to formulators: The compilation of safety data sheets (SDSs) required the use of substance information, also on RMMs, already before REACH came into force. However, under REACH the OCs and RMMs may be described more precisely and quantitative information on efficiencies of emission and exposure reduction may have to be processed by the formulator.

The ECHA DU guidance should provide respective support to formulators. Chapter 14 “Information on preparations to be delivered by formulators” describes the legal obligations and outlines a workflow to structure and support the collection, processing and use of information on CoU to develop SDSs and other information for mixtures. In this workflow a critical component approach (CCA) is mentioned but it has never been further described in the ECHA guidance documents.

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<sup>1</sup> I.e. safety data sheet (SDS), exposure scenario(s) (ESs) and/or information according to Article 32

<sup>2</sup> E.g. results of DU chemical safety reports (DU CSRs) for substances, testing of mixtures



The method “DPD<sup>+</sup>” was developed by CEFIC<sup>3</sup> based on a first proposal by two of its sector associations (ESIG and FEICA) and industry, the EU Commission and ECHA discussed it at a workshop in May 2008. CEFIC states that DPD<sup>+</sup> is one way of implementing the workflow on preparing information for mixtures outlined in ECHA’s downstream user guidance.

## 1.2 Aims of the project

The first aim of the German UFOPLAN project “Consolidation of Information for Mixtures under REACH” was to evaluate whether the consolidation of information for mixtures using DPD<sup>+</sup>

- ensures that all potential environmental risks are correctly covered,
- supports the formulator in efficiently identifying the operational conditions (OCs) and risk management measures (RMMs) that ensure safe use of all substances in the mixture,
- leads to the derivation of adequate (understandable, meaningful and practically implementable) information to the end-users of the mixture.

The second aim of the project was to propose how an appropriate method for the consolidation of information for mixtures could be developed involving either

- the (potentially necessary) improvement of DPD<sup>+</sup> or
- the outline of an alternative approach.

The project was performed by Ökopol between 11/2010 and 10/2011 as desk research. It only concerned environmental risks and information; occupational and consumer aspects were not considered.

## 1.3 Structure of the report

This report describes the evaluation of the DPD<sup>+</sup>-method by CEFIC, which aims to support formulators in consolidating information on substances in the mixtures they produce.

In Chapter 2 the legal obligations of formulators with regard to forwarding information with their products are discussed. Chapter 3 outlines which information is provided to the formulator with the input materials and which information is publicly available to him, in addition. Chapter 4 contains a compilation of approaches towards the assessment of mixture toxicity and discusses chances and challenges of including these in the consolidation process by formulators as voluntary action. Chapter 5 describes the assessment of available methods to assess mixtures with the aim of developing risk management measures for safe use.

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<sup>3</sup> CEFIC: “REACH: Exposure scenarios for preparations - Methodology for the identification of substances that represent the dominant risks to human health and/or the environment and the drivers for risk management measures”, June 2009; [http://www.cefic.org/Documents/IndustrySupport/ES\\_for-preparations-DPD+methodology.pdf](http://www.cefic.org/Documents/IndustrySupport/ES_for-preparations-DPD+methodology.pdf)

In Chapter 6 the DPD<sup>+</sup>-method, as interpreted by the consultant, is described. The different steps for evaluating DPD<sup>+</sup> (analysis of the classification and labelling system, the scope of exposure assessment according to ECHA, the relevance of physico-chemical properties) are described in Chapter 7. Chapter 8 contains an analysis of EU risk assessment reports. In Chapter 9, the main limitations of DPD<sup>+</sup> with regard to the consolidation of information on mixtures are summarized. The results of a theoretical exemplification of the use of DPD<sup>+</sup>, an improved approach of DPD<sup>+</sup> and an alternative approach for consolidating risk information are summarized in Chapter 10. Chapter 0 contains recommendations for further activities.

An executive summary outlining the main project results is published separately.

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## 2 LEGAL OBLIGATIONS OF THE FORMULATOR ACCORDING TO REACH

The description of a formulator's legal obligations is not complete but only concerns duties related to information on mixtures. It is described which type of information must be forwarded to the customers (downstream users) and which specific requirements are defined by REACH regarding the consolidation of substance information for mixtures.

### 2.1 Providing safety data sheets

REACH Article 31 requires formulators to provide safety data sheets (SDSs) of mixtures to their customers according to REACH Annex II, in case the mixture meets the criteria for classification as dangerous<sup>4</sup>. Additionally, SDSs are to be provided on request of customers if mixtures contain at least one substance:

- posing hazards to human health or the environment is present in the mixture in individual concentrations of  $\geq 1$  % by weight for non-gaseous and  $\geq 0.2$  % by volume for gaseous mixtures or
- fulfilling the PBT/vPvB criteria or being listed on the candidate list for authorization is present in the mixture in individual concentrations exceeding 0.1% for non-gaseous mixtures or
- with EU occupational exposure limits (OELs) is present in the mixture.

An SDS is not required if the mixture is sold to the general public and provided with sufficient information to enable safe use (e.g. on the label or packaging) except a downstream user or distributor requests one.

### 2.2 Providing information in case an SDS is not required

REACH Article 32(1) requires formulators to communicate information with mixtures for which no SDS is required if it contains substances

- which are to be authorized; in this case information on the conditions under which the mixture may be applied if an authorization has been granted (otherwise substance may not be used) have to be forwarded;
- that are restricted; in this case information on the details of the restrictions have to be forwarded;
- for which other information is necessary to enable the user to implement safe use, including risk management measures (RMMs).

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<sup>4</sup> Classification as dangerous according to Directive 1999/45/EC.

If any of the above applies, the registration number of the substance for which information is communicated must be provided as well. In the following this set of information is called as “Article 32 information”.

### 2.3 Providing information on the conditions of use

A formulator has to “include relevant exposure scenarios (ES), and use other relevant information, from the SDS<sup>5</sup> supplied to him when compiling his own SDS for the identified uses.” The REACH text is not fully clear with regard to which information should be used in which manner and in which form information on operational conditions (OCs) and risk management measures (RMMs) should be forwarded.

The ECHA guidance on information requirements and chemical safety assessment (IR/CSA guidance) specifies in part G that the formulator has several options to forward information:

- ESs of individual substances received as such,
- consolidated information for the mixture in form of an ES for the mixture,
- individual ESs and a consolidated ES for the mixture,
- inclusion of information in the SDS of a mixture.

This means that formulators are required to use the information from SDSs and ESs received with their input materials to develop information on their products. They are free to decide in which form (integrated into SDS, as ES etc.) they provide that information.

If a formulator prepares a downstream user chemical safety report (DU CSR<sup>6</sup>) for the substances in his mixtures, he is to ensure that the information in his SDS is consistent with the information in his CSR for the substances and the relevant ESs for the substances are attached (REACH Article 37(4)).

If a formulator prepares a DU CSR for his mixture it is sufficient if he ensures consistency of the SDS with the respective DU CSR for the mixture and not with all individual CSRs for the substances (Article 31(2)). The relevant ES(s) developed in the DU CSR for the mixture are to be attached to the eSDS<sup>7</sup>.

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<sup>5</sup> REACH Article 31 (7). In the legal text, any downstream user is explicitly obliged to use exposure scenarios and information that is communicated to him in the SDS (shall). It is assumed that – as in relation to many other REACH provisions, other relevant information that he receives e.g. according to Article 32 in case no SDS is required should also be taken into account. This is supported by the requirement to update SDSs upon receipt of any “[...] new information which may affect the risk management measures, or new information on hazards [...]” according to Article 31(9).

<sup>6</sup> According to Article 37 (4) a DU CSR is required for a substance for any use advised against and any use outside the conditions communicated in the SDS or the ES. The DU is exempted from that obligation, a) if he doesn't have to provide an SDS for the mixture, b) his supplier (registrant) is not required to complete CSR in acc. with Article 14, c) the DU uses less than 1 ton per year of the substances or mixture, d) the DU recommends or implements as a minimum the conditions communicated to him (scaling), e) the substance is contained below concentrations set out in REACH Article 14(2) or f) he uses the substances for PPORD and complies with respective obligations.

<sup>7</sup> REACH does not define any details of the requirements to DU CSRs for mixtures. In analogy to CSRs for single substances it is assumed that whenever a (DU) CSR is prepared, an ES must be attached to the SDS supplied by the actor having carried out the assessment (Article 31(7)).

This means that formulators that carry out DU CSRs for substances have to attach the ESs for the substances; formulators that carry out a DU CSR for a mixture have to attach the ES for the mixture to their SDS in addition to including relevant and consistent information in the main body of the SDS.

REACH Article 37(6) states that downstream users (DUs) – who are exempted from the obligation to make a DU CSR because they use less than 1 t/a of the substance or mixture – are nevertheless responsible to identify and communicate relevant information to adequately control risks in the SDS, if one is prepared.

If information according to Article 32 is supplied with the mixture, formulators have the obligation to use available information on RMMs in order to recommend appropriate information to the DUs according to Article 37(5).

## 2.4 Consolidation of information for mixtures

The term „consolidation of information“ is not used in REACH but has evolved in the discussion on the DU obligations. It is used to address the process of using information received from suppliers of substances or mixtures (SDS, ES, Article 32 information) or generated by the DU (e.g. results of DU CSRs for substances, testing of mixture) to select the relevant information on operational conditions (OCs) and risk management measures (RMMs) to allow the customers to recommend and implement measures that ensure adequate control of risks.

In contrast to a chemical safety assessment (CSA) and according to the understanding of the term in this project, for consolidation of information the PEC/PNEC<sup>8</sup> relationships of the substances in the mixture don't have to be calculated; i.e. no risk characterisation is performed. This is because the formulator uses information he receives and assumes the conclusions in the CSR of his supplier, which are forwarded to him in the ES or eSDS are correct. Hence it is ensured that the PEC/PNEC-ratio still remains under 1, if the information he forwards corresponds to or remains within the borders of the received information. The formulator may of course check the result of the consolidation processes by making an own risk assessment.

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<sup>8</sup> The quotient of the predicted environmental concentration and the predicted no-effect concentration of a substance is also called risk characterisation ratio (RCR).

Table 2.1: Overview of obligations to formulators under REACH related to providing information with mixtures<sup>9</sup>

| Information for mixture to be provided                                      | Conditions defining type of information to forward   | Type of information to forward   | Information to include from  | Action to take  |
|---|--|--|--|---|
| No information  | Mixture not classified as dangerous AND no substances posing risks OR having Community wide OELs OR fulfilling PBT/vPvB criteria or being on the candidate list (Article 31(1+3))  | None   | None   | None<br>Best practice: Forward information on substances which are not classified but could pose risks or give rise to concern  |
| Consumer information  | Mixture is sold to general public AND appropriate information is provided, EXCEPT DUs or distributors request other type of information (Article 31 (4))   | Guidance on safe use: OCs and RMMS if necessary to ensure control of risks                                 | Received SDS, ES, DU CSR   | No requirements defined!<br>Best practice: Assess and consolidate received information appropriately, provide respective advice on label / packaging / instructions   |
| Information for DU in case a safety data sheet is not required (Article 32) | Mixture is not classified as dangerous AND the mixture contains substances as such or in mixtures, for which authorization is necessary or granted OR restrictions exist OR information to take appropriate RMM exist (Article 32).  | Article 32 information and registration number(s) of respective substances                                 | Received Article 32 information DU CSR<br>Additional information on mixture, if relevant <sup>10</sup> | Provide information on authorization / restrictions from Article 32 information received, ensure compliance of mixture and consolidate if needed<br>Best practice: In addition: consolidate information on OCs and RMMS to adequately control risks |
| Safety data sheet according to Article 31                                   | Mixture is classified as dangerous OR a SDS is requested AND the mixture contains substances posing risks in concentrations $\geq 1\%$ w/w (non-gaseous) or $\geq 0.2\%$ vol% (gaseous) OR having Community wide OELs OR fulfilling PBT/vPvB criteria or being on the candidate list (Article 31(3)) | Information ensuring adequate control of risk consistent with information obtained or own DU CSR conducted | Received SDS, ES<br>Additional information on mixture, if relevant                                     | Compile information to adequately control risks and forward in appropriate form<br>Best practice: consolidate all information.  |
| Extended safety data sheet  | c.f. above AND DU CSR is carried out for substance in the mixture or the mixture as such   | c.f. above AND exposure scenario(s) derived from the DU CSR(s)   | Received SDS, ES, additional information and any available information to carry out DU CSR             | Attachment of ESs as derived from DU CSR;<br>Consistency with SDS and other attached ESs to be ensured  |

<sup>9</sup> The term "Best practice" in the column "Action to take" outlines the optimal case, in which the formulator would invest all possible efforts and resources in providing best information to his customers. These actions exceed the legal obligations and are hence voluntary.

<sup>10</sup> This may be the case if e.g. the mixture is provided as powder (risks from dust).

### 3 INFORMATION AVAILABILITY FOR THE FORMULATOR ACCORDING TO REACH

REACH Annex II<sup>11</sup> defines which information is to be provided to downstream users (DU), including formulators with the safety data sheet. Further explanation is given in the ECHA draft guidance document on safety data sheets (SDS)<sup>12</sup>. Under REACH, safety data sheets with attached exposure scenarios (ES) are called extended safety data sheet and are abbreviated eSDS. In general, the formulator has to forward the same type of information he receives from his suppliers. The following chapters discuss which information is received and should be provided either in the main body of the SDS and / or in form of an attached ES.

#### 3.1 Composition/Information on ingredients ; SDS section 3

According to REACH Annex II, substances among others<sup>13</sup> presenting a human health or environmental hazard in the meaning of Directive 67/548/EEC<sup>14</sup> (Dangerous Substances Directive – DSD) and contained above the respective thresholds for consideration are to be listed in Section 3 of the SDS with their individual concentrations or concentration ranges.

The thresholds for consideration are generically defined in Directive 1999/45/EC (Dangerous Preparations Directive - DPD) and the Regulation (EC) No 1272/2008 (CLP-Reg.) or may be specific, and provided separately (in Annex VI of the CLP-Reg.)<sup>15</sup>.

PBTs/vPvBs need to be considered if they are contained in concentrations above 0.1%. If lower (specific) concentration limits are defined or if M-Factors<sup>16</sup>

<sup>11</sup> Amended by Regulation (EC) No. 453/2010

<sup>12</sup> ECHA: Guidance on the compilation of safety data sheets; 4th draft; Helsinki, July 2011; available at: [http://guidance.echa.europa.eu/docs/default\\_documents/fourth\\_draft\\_sds\\_guidance\\_july\\_2011.pdf](http://guidance.echa.europa.eu/docs/default_documents/fourth_draft_sds_guidance_july_2011.pdf)

<sup>13</sup> In addition, substances for which occupational exposure limit values exist and substances meeting the criteria of Annex XIII as PBTs/vPvBs contained in individual concentrations above 0.1% vol/vol have to be identified.

<sup>14</sup> Directive 67/548/EEC (DSD) uses the term "dangerous" and defines the respective categories whereas Regulation (EC) No 1272/2008 (CLP-reg.) introduces the term "hazardous" and defines respective hazard categories. The provisions of REACH normally relate to "dangerous according to Directive 67/548/EEC" or – for mixtures – according to Directive 1999/45/EC. Therefore, in the following the term dangerous is used as well.

<sup>15</sup> According to Annex II of REACH, Section 3.2, for mixtures classified as dangerous the following need to be considered: limit concentrations according to Annex I of Directive 67/548/EEC (Annex VI of the CLP-regulation); Table 3.3, Part B of Annex II, Part B Annex III or Annex V of Directive 99/45/EC; substances, for which occupational exposure limit values exist or which are PBTs/vPvBs contained in concentrations above 0.1% w/w. For mixtures, which are not classified, substances need to be considered, if they are contained in concentrations above 1% if they pose a hazard to human health or the environment or if they are PBTs/vPvBs in concentrations above 0.1%.

<sup>16</sup> M-factors are used in the environmental classification of substances according to the CLP-Reg. if substances have a higher aquatic toxicity than 1 mg/l (LC50) or 0.1 mg/l (NOEC).

are to be applied, these (lower) limits are to be used to decide which substances have to be identified. The identity of substances contained in the mixture in lower concentrations than any of the defined thresholds doesn't have to be disclosed in the SDS. Hence, the information is "lost" and the formulator has no legal basis to request that information from his supplier.

For non-classified mixtures information has to be provided according to Article 32; i.e. only if a mixture contains substances which are subject to restriction(s), have to be authorized or require specific risk management measures (RMMs). Information on PBTs/vPvBs is to be forwarded as well. Furthermore, information may be forwarded on a voluntary basis, e.g. if substances with EU occupational exposure limit values are contained in the mixture.

The knowledge on the composition of a mixture is the basis for any work on consolidation of information for mixtures used as input materials to produce another mixture. This is because the individual components must be considered and not the mixture as such.

The thresholds for consideration<sup>15</sup> legally limit the possibilities of formulators to obtain information; i.e. a formulator has no means to request the identity of components in mixtures below the consideration thresholds. The consideration thresholds have been agreed between experts as borderline for "negligible risk contributions"; i.e. it is assumed that substance contained in mixtures in lower concentrations don't have to be considered in the identification of a mixture's hazardous properties / classification. Consequently, the consideration thresholds should be used as cut-off limits for taking substance in mixtures into account in the assessment and consolidation of information for mixtures.

Formulators using mixtures as input materials may receive SDSs with consolidated information on the substances in the mixtures. It may not always be obvious, which information applies to which ingredient. It may be particularly difficult to identify which component in the mixture has triggered the need for a specific RMM. This is a challenge that can be met either by requesting the substance ESs from the suppliers, if available, or by assuming that all information applies to any of the substances contained in the mixture.

## **3.2 Exposure controls / personal protection; SDS section 8**

### **3.2.1 Information from hazard assessment**

According to REACH and the draft ECHA guidance on safety data sheets, in Section 8 of the SDS, all PNECs<sup>17</sup> "[...] applicable to the exposure scenarios in any required annex(es) to the SDS for a specific substance or mixture [...]" can be listed<sup>18</sup>. It is also mentioned that non-applicable PNECs should be removed / not listed. In an exemplary table in the ECHA guidance, possible PNECs to list include PNECs for water (pelagic, marine), air, soil, sediment (pelagic,

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<sup>17</sup>Predicted No Effect Concentration; concentration of the substance, below which no adverse effect is expected

<sup>18</sup> ECHA guidance on the compilation of safety data sheets, 4<sup>th</sup> draft July 2011 p. 66.



marine) and the sewage treatment plant (STP); hence any relevant protection target should be covered.

Hence, it can be assumed that only those PNECs which are relevant for safe handling and use and/or for determining the appropriate conditions of use and risk management measures should be quoted. This may also vary for different customers.

Regarding environmental exposure controls few specific information is given in REACH and the draft ECHA guidance on SDSs; no specific provisions are given for mixtures. In analogy to substances, it can be assumed that the RMMs needed to ensure adequate control have to be summarized, including particularities on the operational conditions of use (OCs), if identified in a chemical safety assessment (CSA), as they are essential in the assessment of safe use.

### 3.2.2 Information from exposure assessment

The information used in the release estimation and exposure assessment forms part of the ES and is hence to be forwarded to the formulator in form of OCs and RMMs. The information is normally provided in numeric values:

- Input amount of substance to the process (fraction at main source:  $F_{\text{main source}}$  amount used at site per day or year:  $M_{\text{spec}}$  etc.)
- Number of emission days ( $T_{\text{emission}}$ )
- Efficiency of risk management measures ( $\text{RMM}_{\text{eff}}$ )

The registrant has to identify and recommend RMMs necessary to ensure safe use of substances as such or in mixtures. As a minimum he must specify the efficiency for emission reduction to be achieved. The forwarded information must be sufficient for the DU to compare whether or not the conditions at his site comply with the ES or information in the eSDS he receives.

Furthermore, the formulator receives standardized information on the processes covered by the ES concerning:

- Lifecycle stage – for the formulator consolidating information for mixtures information on the downstream use and the service life as well as the waste stage are relevant;
- Level of containment of processes (open, closed, open-closed);
- Intended technical fate of the substance (processing aid, reactive processing aid, reaction on use, no inclusion in matrix, inclusion into/onto matrix, removing from matrix, losses with matrix during article processing);
- Dispersion of emission sources (industrial, wide dispersive);
- Indoor or outdoor use of the substance;
- Release promotion during service life (none, low, high);
- Volume flow rate of receiving water and municipal sewage treatment plant and/or dilution rates.

Apart from the information on OCs and RMMs forming the basis of release estimations and exposure assessments, no additional information from the CSA

has to be provided by the registrant. The following information is available in the CSA but not necessarily communicated:

- release factors to the environment (RF<sub>air</sub>, RF<sub>water</sub>, RF<sub>soil</sub>) used to estimate the emitted amount of a substance;
- emission rates to the local<sup>19</sup> [kg/d] and the regional environment<sup>20</sup> [t/a], which are the result of the emission estimation;
- predicted environmental concentrations (PECs) for all relevant compartments in the local and regional environment;
- risk characterization ratios (RCRs) derived by dividing the PECs by the PNECs. Only RCRs < 1 indicate safe use. If RCRs exceed the value of 1, the use cannot be communicated as safe and either the CSA must be refined, potentially resulting in the recommendation of different OCs or stricter RMMs or the use must be advised against.

### 3.2.3 Information on RCRs and types of effects

The risk characterization ratios (RCRs) are the core indicators for adequate control of risk in the CSA. RCRs should be derived for all relevant environmental compartments. If a complete assessment is performed the following RCRs should be available for all relevant life-cycle stages of the substance:

- RCR<sub>water</sub> (freshwater and marine); local and regional
- RCR<sub>sediment</sub> (freshwater and marine); local and regional
- RCR<sub>soil</sub>; local and regional
- RCR<sub>STP</sub>; local
- RCR<sub>predatos</sub> (freshwater, marine); aquatic and terrestrial food chains

For the air compartment, the ECHA guidance on risk characterization specifies that a qualitative assessment of abiotic effects should be carried out and ozone depletion is given as one example. Furthermore, an assessment of biotic effects to plants could be carried out. The ECHA guidance does not mention ozone formation, global warming or long range transport as abiotic effect to be considered in the assessment.

RCRs are normally not communicated to DUs but are available at the registrants for all substances, for which a CSA has been carried out. RCRs directly reflect the anticipated risk level. They could be a perfect indicator for comparing the risk levels resulting from different substances. However, in most cases RCRs will not be available to the formulator, because registrants may not have performed a chemical safety assessment. Even if a CSA was available, it is questionable if RCRs would be readily communicated down the supply chain.

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<sup>19</sup> For industrial sources at local scale, direct emissions to air and wastewater (100% connection to STP) are determined, because industrial soil is not a protection target. For wide dispersive uses at local scale only emissions to water and the STP are assessed. Due to partitioning in the environment, PECs are calculated for all compartments.

<sup>20</sup> For both industrial and wide dispersive use, direct emissions to air, surface water, STP and soil are determined at regional level.

### 3.3 Physical and chemical properties; SDS section 9

Information on physico-chemical (PC) properties is to be given in Section 9 of the SDS. Many PC-properties are derived from testing of the mixture. However, most parameters relevant for the assessment of environmental exposures are relevant only with regard to the individual substances. In Annex II of REACH it is not specified if the boiling point and relative density should be provided for substances or for the mixture. The following PC properties are specified in this regard:

- vapour pressure → refers to the most volatile substance
- water solubility → substance specific information recommended
- $\log K_{ow}$  → substance specific information is recommended

### 3.4 Ecological information; SDS section 12

REACH Annex II does not specify if the information on environmental toxicity in the SDS should relate to the mixture as a whole or the individual components. Data on mobility (including mobility in soil based on experimental data or modelled from  $\log K_{ow}$ ), bioaccumulation, persistence and degradability data shall be given, where available and appropriate for each of the components in the mixture.

The results of any PBT/vPvB assessment of the constituents in the mixture shall be given and forwarded as well as information on other adverse effects such as environmental fate, photochemical ozone creation potential, ozone depletion potential, endocrine disrupting potential and/or global warming potential.

### 3.5 Public access to information

According to REACH Article 119 environmentally relevant information on substances will be published in ECHA's dissemination data base. That means formulators knowing the composition of their mixtures and the identity of the individual components can retrieve the following information from the data base, if it is not provided by the supplier:

- classification and labelling;
- physicochemical data and information on environmental fate;
- results of ecotoxicological studies (LC/EC/IC);
- any predicted no-effect concentration (PNEC) established in accordance with Annex I;
- guidance on safe use according to Annex VI, Sections 4 and 5;

PNECs will only be available for those endpoints that can be derived based on the available information (c.f. Section 0) and with regard to the information requests of REACH-legislation Annex VII – X. Hence, for substances registered in amounts below 10 t/a no PNEC will be available. Information to derive the

PNEC will also not be available, because only two tests are required for this tonnage band and three are needed for estimating the PNEC.

### 3.6 Conclusions on information availability

Formulators know the identity of their input materials if the use:

- Substances as such (classified or not classified as hazardous<sup>21</sup>);
- Classified substances contained in classified mixtures<sup>22</sup>, if they are contained above the consideration thresholds and are hence identified in the SDS;
- Classified substances contained in non-classified mixtures<sup>22</sup>, if information according to Article 32 has to be forwarded for them or information can be requested by the DUs.

Methods for consolidating information on mixtures should not require the formulator to take substances into account, for which he is not (legally) able to obtain information on their identity, i.e. classified substances in mixtures contained in concentrations below the consideration thresholds and non-classified substances contained in mixtures. This is because they are not likely to significantly contribute to environmental risks and the efforts to obtain information are disproportionate.

Formulators do have access to substance information for known components (CAS-Number, name etc.) they use. Information they can obtain from their suppliers or the ECHA data base include the results of testing and derived PNEC values. No information is available to him on substances which are not registered and not identified in the SDS. For these substances classification and labelling information may be accessible, as there is no tonnage threshold for classification.

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<sup>21</sup> As substances are to be classified according to the CLP-Regulation, here the term hazardous is used. Mixtures only have to be classified according to the CLP-Regulation by 2015 and therefore, the term dangerous is used.

<sup>22</sup> Except the identity of substances has been claimed confidential

## 4 APPROACHES FOR THE ASSESSMENT OF MIXTURES

The following Sections represent only an initial screening of information on the availability of methods for mixture toxicity assessment and their potential use under REACH. It should be noted, that currently there is no legal obligation under REACH to assess the mixture toxicity and/or to communicate respective information along the supply chain. Also the guidance documents barely mention that mixture toxicity should be considered. In order to further assess the feasibility of including mixture toxicity assessments in the REACH procedures the Umweltbundesamt commissioned a separate project.<sup>23</sup>

In the classification of mixtures, formulators do already take account of joint action via the additivity rules of the Preparations Directive. On a voluntary basis they could also include information from assessments of the joint action<sup>24</sup> of substances in a mixture in their consolidation process on information on the safe conditions of use. In the following, approaches for assessing the toxicity and potential risks of mixtures are briefly characterized.

### 4.1 Scientific background on mixture toxicity

In the scientific debate, two models are established to predict mixture toxicity on the basis of available data on single substances: Concentration Addition (CA) and Independent Action (IA). Both models require information on the toxicity of the components in the mixture. If no information on the toxicity of a mixture's components is available, testing the mixture as a whole is the only way of predicting its toxicity.

The model of Concentration Addition as first developed by Loewe and Muischnek assumes a direct relationship between the concentration of all individual components of a mixture and the effect on the organisms. In other words, CA acts on the assumption that the components of the mixture behave like dilutions of the same substance, only differing in their relative potencies. Therefore, traditionally a similar mode of action of the components is seen as prerequisite.

The toxicity of a mixture is determined according to the CA model by an addition of the quotients of the toxicity values (e.g. L(E)C values) and the respective concentrations of all contributing substances. This quotient is also known as

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<sup>23</sup> UFOPLAN project "Mixtures in the environment – development of assessment strategies for the European chemicals regulation REACH" (FKZ 3711 63 429) commissioned to a project cooperation of Öko-Institut, Ökopol and Fobig to be performed between 01/2012 and 6/2013.

<sup>24</sup> Joint action in this context means combined effects of different substances, additive effects or interaction between substances as there may be antagonism or synergism.

toxic unit (TU). In principle all components are considered, regardless of their concentration.

| Concentration Addition (CA)          | Independent Action (IA)                       |
|--------------------------------------|---|
| Loewe & Muischnek 1926               | Bliss 1939                                    |
| $\sum_{i=1}^n \frac{c_i}{ECx_i} = 1$ | $E(c_{Mik}) = 1 - \prod_{i=1}^n [1 - E(c_i)]$ |
| Similar action                       | Dissimilar action                             |

Figure 1: Comparison of mixture toxicity assessment approaches

The model of Independent Action (IA) is based on the idea that components of a mixture have dissimilar modes of action and act independently on different targets, but cause a common integral biological effect. In contrast to CA the calculation of mixture toxicity is based on effects and not effect concentrations. Hence, according to IA components below their no-effect level would not contribute to the toxicity of the mixture as a whole. However, studies have shown that mixtures produce toxic effects even if all components are below their threshold values.

It has been demonstrated that CA is also applicable for mixtures that are not entirely composed of strictly similar acting substances but also contain dissimilar acting substances. Moreover, the CA model most often gives more conservative and therefore more precautionary results. Therefore, it has been proposed to be used as default concept. However, the model IA may still be applicable for cases of strictly dissimilar acting substances.

With regard to the applicability of the methods it is stated:

“The practical relevance of independent action for the assessment of mixture effects has been called into question on the basis of considerations of biological organization. The principle of strictly independent events may only rarely be relevant due to converging signalling pathways and inter-linked subsystems. For these reasons, dose (concentration) addition has been deemed more broadly applicable, and has even been termed the “general solution” for mixture toxicity assessment.”<sup>25</sup>

The two models - Concentration Addition (CA) and Independent Action (IA) - can be used to predict the toxicity of mixtures with a reasonable precision<sup>26</sup>. They are based on the assumption that the components of the mixture don't interact; i.e. they don't react with another and thereby modify the (eco-)toxicity. Several challenges have been identified by the authors of two review reports (UBA report<sup>27</sup> and EU report<sup>25</sup>) relating to the application of the methods in the scientific context.

<sup>25</sup> The School of Pharmacy University of London (ULSOP): State of the Art Report on Mixture Toxicity, Final Report, Contract number 070307/2007/485103/ETU/D.1, December 2009.

<sup>26</sup> According to UBA report, results from comparing predictions with experimental data differ in average by the factor 2. Underestimations are observed mainly for biocidal products and mixtures of metal compounds. The reasons for stronger effects than predicted are not explained yet.

<sup>27</sup> Bericht über den Stand der Ergebnisse zum Arbeitspaket 2.1 „Grundlegende Fragestellungen“ im Rahmen des UBA-Forschungs- und Entwicklungsvorhabens „Ökotoxische Kombinationswirkungen von Stoffgemischen“ FKZ 3709 65 404

According to the EU report<sup>28</sup> on mixture toxicity the most studied groups of substances are pesticides, heavy metals, endocrine disrupters, poly-aromatic hydrocarbons (PAHs) and general industrial chemicals. The first groups of substances are either only partly in the scope of REACH (active substances), are to be assessed with specific methods (heavy metals) or are likely to be of high concern (or even Substances of Very High Concern (SVHC) according to Article 57 of the REACH-regulation). This means that the mixture toxicity has been assessed in scientific contexts mostly for substances of very high concern or which don't follow the general risk assessment principles in the EU – regulatory framework. The relevance of the approaches regarding substances used in industrial mixtures may be an issue for future discussion.

#### **4.2 Risk assessments under the existing substances regulation (793/93 EEC)**

Under the existing substances regulation (ESR)<sup>29</sup> substances listed in the European Inventory of Existing Chemical Substances (EINECS) were ranked on four priority lists and assessed by different Member States (MS) in order to identify potential risks. In the context of this regulation, the European Technical Guidance Document (EU TGD<sup>30</sup>) has been developed, which amongst others outlines detailed rules for risk assessment of substances and outlines a set of default values for exposure estimates for the environment. The EU TGD has been the basis upon which EUSES has been programmed. EUSES is a decision-support instrument (software programme), which enables the user to carry out rapid and efficient assessments of the general risks posed by substances to man and the environment. It is intended mainly for initial and refined risk assessments rather than comprehensive assessments. The approaches and rules of the EU TGD have been transferred to the rules and settings of the chemical safety assessment under REACH.

The risk assessments performed under the ESR concerned single substances. Hence, no approaches to mixture toxicity are included in either the assessment reports or the EU TGD itself.

#### **4.3 Assessment of mixtures under different regulatory frameworks**

In the following, regulatory assessment methods are described, which include considerations on joint action of substances in mixtures. Some of these belong to a risk assessment approach under specific legislation.

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<sup>28</sup> State of the Art Report on Mixture Toxicity

<sup>29</sup> COUNCIL REGULATION (EEC) No 793/93 of 23 March 1993 on the evaluation and control of the risks of existing substances.

<sup>30</sup> Technical Guidance Document on Risk Assessment in support of Commission Directive 93/67/EEC on Risk Assessment for new notified substances, Commission Regulation (EC) No 1488/04 on Risk Assessment for existing substances, Directive 98/8/EC of the European Parliament and of the Council concerning the placing of biocidal products on the market. Brussels. Part I - Part IV.

#### 4.3.1 Classification of mixtures (1999/45/EC and (EC) No 1272/2008)

The classification of mixtures is regulated by Directive 1999/45/EC (Dangerous Preparations Directive - DPD) and Regulation (EC) No 1272/2008 (classification and labelling regulation – CLP-Reg.). The classification rules relevant for the consolidation of information related to the environment are briefly outlined in the following. In order to prevent later updating needs of the document, ONLY the rules of the CLP-Regulation are explained.

##### Principles and general issues

The classification of substances is based on their intrinsic hazards.

The classification of a mixture should generally be based on information from testing of a mixture as such, if available. Testing of the ecotoxicity of mixtures would integrate any joint action of its components automatically. Joint action in this context means all consequences of the concurrence of substances in the mixture.

The biodegradation and bioaccumulation potentials are always to be determined for the single substances. An environmental classification based on testing of the mixture is hence possible for acute toxicity and for chronic toxicity if no ready degradability of at least one of the components is assumed or known.

If no information is available on the mixture, several rules can be applied to identify the classification based on analogies and logics (bridging principles, c.f. also Chapter 7.1.3).

If neither test results of the mixture are available nor the bridging principles can be applied the summation method is to be used, which is based on the hazards of the components of the mixture and assumes additivity of effects for the environment.

Apart from the classification for aquatic effects, substances and mixtures may be classified because of their ozone depletion potential. The ozone depletion potential should always be classified based on the individual components.

##### Concentration thresholds for the environment

Annex I of the CLP regulation defines consideration threshold levels above which substances are to be taken into account (0.1<sup>31</sup> or 1% for aquatic toxicity) for the classification of the mixture. Secondly, concentration thresholds are defined above which a component triggers the classification of a mixture<sup>32</sup>. For substances which are very toxic to the aquatic environment (acute and chronic category 1), a multiplication factor is to be used (M-Factor) in classifying a mixture. The M-factor is defined in relation to the L(E)C50-values. Substances with an L(E)C50 of 0.5 mg/l trigger classification with H 400 above concentrations of 0.25%. Substances with a L(E)C50 of 0.05 mg/l trigger classification with H 400 already above concentrations of 0.025% in the mixture

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<sup>31</sup> < 0,1% depending on the M-factor where relevant; i.e. the LC/EC/ErC50 is lower than 0.1 mg/l.

<sup>32</sup>The threshold concentrations of the dangerous preparations directive and the CLP regulation are the same.



(M-factor 10). According to Regulation (EC) No 286/2011 it is also possible to define M-factors based on results of testing the chronic aquatic toxicity (NOECs).

#### Classification for the environment

For the classification of aquatic toxicity (H400 – H413) concentrations of substances in the mixture which are toxic to the aquatic environment have to be added up. Ozone depletion is considered a single substance effect and no concentrations are added.

The classifier may either use the summation or the additivity method or both (in the latter case the strictest classification is to be selected). Both methods imply additivity of effects.

According to the additivity method, the toxicity of a mixture is determined by adding the quotients of the EC50 values [mg/l] and the concentrations [mg/l] of the individual components. The result of the calculation is a predicted EC50 value for the mixture to be compared to the classification thresholds.

$$EC_{50,mix} = \sum (EC_{50,i} / C_i) * C_{\Sigma}$$

$EC_{50,mix}$  = (calculated) test concentration of the mixture at which 50% of the test organisms exposed to it show an effect [mg/l]

$EC_{50,i}$  = test concentration of a component in the mixture at which 50% of the test organisms show an effect [mg/l]

$C_i$  = concentration of the component in the mixture [mg/l]

$C_{\Sigma}$  = concentration of all substances in the mixture contributing to the effect [mg/l]

The summation method requires adding up the (weighted<sup>33</sup>) concentrations of all substances classified in the same category and comparing the resulting concentration to the classification threshold. A multiplication factor (M-Factor) may have to be applied for very toxic substances.

Table 4.1: Mixture classification (acute aquatic toxicity) according to CLP-reg.

| Sum of components, which are classified as: | Mixture classified as |
|---|-----------------------|
| Acute 1 X M ≥ 25%                           | Acute 1               |

Table 4.2: Mixture classification (chronic aquatic toxicity) according to CLP-reg.

| Sum of components which are classified as:                 | Mixture classified as: |
|--|------------------------|
| Chronic 1 X M ≥ 25%  | Chronic 1              |
| (M X 10 X chronic 1) + chronic 2 ≥ 25%                     | Chronic 2              |
| (M X 100 X chronic 1) + (10 X chronic 2) + chronic 3 ≥ 25% | Chronic 3              |
| Chronic 1 + chronic 2 + chronic 3 + chronic 4 ≥ 25%        | Chronic 4              |

<sup>33</sup> A factor of 10 or 100 is applied when substances of a more severe classification category contribute to the classification in a less severe category. Substances classified as chronic category 1 are weighted by the factor 10 when a classification in category chronic 2 is checked and by the factor 100 for the category chronic 3. See also Table 4.2 with the summation formulas.

#### 4.3.2 PBT/vPvB assessment of multi constituent and UVCB substances according to ECHA<sup>34</sup>

Multi constituent substances (MCS) and Substances of Unknown or Variable Composition, Complex Reaction products and Biological materials (UVCB) are constituted of single substances which are regarded as one substance according to the rules for substance identification under REACH<sup>35</sup>.

However, these types of substances could also be regarded as mixtures of different constituents. When determining the toxic properties of these substances, e.g. in a PBT assessment, joint action of the various constituents may be considered. The respective approaches were briefly analysed to check if this is the case.

A MCS / UVCB is treated as PBT/vPvB containing substance if it consists of one or more constituents with PBT/vPvB properties in individual concentrations  $\geq 0.1\%$  (w/w)<sup>36</sup>. Hence, for this type of hazard, the content of individual components is relevant and no concentration addition of components takes place. Consequently in general all constituents with a concentration of  $> 0.1\%$  in the substance need to be considered.

The constituents of UVCB or MCS may be blocked (grouping) for testing, modelling and data evaluation. The ECHA guidance provides rules for determining persistence and bioaccumulation for UVCB substances consisting of homologous structures<sup>37</sup> and those<sup>38</sup> that don't. For multi constituent substances, no respective methods are explained. The toxicity should be determined as concentration response depending on the bioavailability of the individual constituents. Substance testing is only accepted for classification but regarded as problematic for the T-assessment (lethal loading test procedure) and therefore, the use of models is recommended (in addition).

In summary according to the PBT/vPvB assessment approach of MCS/UVCBs the hazardousness of the "substance mixture" is determined based on the individual concentrations of the components; no joint action of the components is assumed. However, this approach is very specific as it concerns the PBT/vPvB assessment of complex substances. It is therefore not suitable to deduce general statements on the assessment of mixture toxicity.

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<sup>34</sup> ECHA: guidance on information requirements and chemical safety assessment (IR/CSA), Part C, Helsinki, May 2008; and ECHA: guidance on information requirements and chemical safety assessment, Chapter R 11, Helsinki, May 2008 available at: [http://guidance.echa.europa.eu/guidance\\_en.htm](http://guidance.echa.europa.eu/guidance_en.htm)

<sup>35</sup> ECHA guidance: Guidance for identification and naming of substances under REACH, Helsinki, June 2007. Available at: [http://guidance.echa.europa.eu/docs/guidance\\_document/information\\_requirements\\_r11\\_en.pdf?vers=20\\_08\\_08](http://guidance.echa.europa.eu/docs/guidance_document/information_requirements_r11_en.pdf?vers=20_08_08)

<sup>36</sup> According to the IR/CSA guidance, chapter R 11, the threshold of 0.1% may be increased based on arguments relating to the use and emission pattern as well as the relevance of risk expected up to a maximum of 10% of the total amount of constituents with PBT/vPvB properties in the substance, if the total amount of these substances remains below 1 t/a.

<sup>37</sup> If in whole substance testing 60% are proven to be readily degradable, substance should not be regarded as persistent.

<sup>38</sup> Case-by-case assessment based on the individual groups of substances and or assessment by using QSARs

#### 4.3.3 Toxicity assessment of plant protection products (according to Regulation 1107/2009)

According to the Regulation on Plant Protection Products<sup>39</sup> active substances can only be used in plant protection products after authorization by Member States. Authorization can be granted for products that contain only active substances which have been approved for use at EU level, following a scientific risk assessment involving among other the European Food Safety Authority (EFSA) and respective conclusions and actions on risk management, if necessary.

The regulation requires an assessment of “combination effects”, in case there is evidence from information that the toxicity of the mixture may exceed that of the active substances in the mixture. Combined effects can either be assessed based on testing of the mixture or by the concept of Concentration Addition of the relevant components in a mixture; i.e. related to the environment the components contributing to the aquatic toxicity. These components may be weighted by specific (multiple action) factors.

#### 4.3.4 Toxicity assessment of biocidal products (according to Directive 98/8/EC)

According to the Biocides Directive<sup>40</sup> active substances are to be assessed at EU level using the EUTGD and based on information compiled by the manufacturer of the active substance. Biocidal products are to be evaluated at Member State level based on a dossier submitted by the formulator of the biocidal product before they are authorized for placing on the market. For the assessment of biocidal products (mixtures) technical notes for guidance have been developed (TNSG<sup>41</sup>). According to the Biocides Directive, “synergistic effects” of active substances with co-formulants should be taken into account in the risk assessment. The TNSG provide the equation for calculating a respective risk characterization ratio for the mixture:

$$RCR_{mix} = \sum [PEC_i / PNEC_i]$$

$RCR_{mix}$  = Risk characterization ratio of the mixture

$PEC_i$  = Predicted environmental concentration of the individual substances

$PNEC_i$  = Predicted no effect concentration of the individual substances

This equation indicates that Concentration Addition is the underlying model for the risk characterization in the context of biocides.

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<sup>39</sup> REGULATION (EC) No 1107/2009 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 21 October 2009 concerning the placing of plant protection products on the market and repealing Council Directives 79/117/EEC and 91/414/EEC

<sup>40</sup> DIRECTIVE 98/8/EC OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 16 February 1998 concerning the placing of biocidal products on the market. A proposal for a new regulation on biocides is currently in the process of being decided at EU level.

<sup>41</sup> The different guidance documents are available at: <http://ecb.jrc.ec.europa.eu/biocides/>

#### 4.3.5 Hydrocarbon Block Method–ECHA guidance and EU TGD

The hydrocarbon block method is introduced in the EU TGD, part II Appendix IX, and is also part of the ECHA guidance Part R 11 on PBT assessment (Appendix 11-3) to identify the risks from petroleum substances. The principle of concentration addition is applied as described for biocidal products by adding the predicted environmental concentrations and the predicted no effect concentrations of individual substance fractions that are similar in structure and effects. The equation for calculating the risk characterization ratio is

$$RCR = \sum [PEC_i / PNEC_i]$$

*RCR = Risk characterization ratio of the petroleum substance*

*PEC<sub>i</sub> = Predicted environmental concentration of the individual constituents of the substance*

*PNEC<sub>i</sub> = Predicted no effect concentration of the individual constituents of the substance*

#### 4.3.6 Other EU – legislation on chemicals

Under the cosmetics legislation<sup>42</sup> no requirements exist to carry out an environmental risk assessment for the components of products or the mixtures as such.

The legislation regulating pharmaceuticals<sup>43</sup> requests applicants for the product authorization to make an assessment of environmental risks. Reference is made to assessment methods of the EU Commission<sup>44</sup>, in particular related to genetically modified organisms. No additional or new methods for the assessment of mixture toxicity are established or described.

Legislation on detergents<sup>45</sup> only considers the degradability of substances but not their toxicity. Hence, no additional information on mixture toxicity is contained.

### 4.4 Methods to determine mixture toxicity at international level

#### 4.4.1 International program on chemical safety

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<sup>42</sup> REGULATION (EC) No 1223/2009 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 30 November 2009 on cosmetic products

<sup>43</sup> Directive 2001/83/EC of the European Parliament and of the Council of 6 November 2001 on the Community code relating to medicinal products for human use and its amendment by Directive 2004/27/EC of the European Parliament and of the Council of 31 March 2004

<sup>44</sup> European Commission: "The rules governing medicinal products in the European Community, Volume III" and its supplements: "Guidelines on the quality, safety and efficacy of medicinal products for human use" available at [http://ec.europa.eu/health/documents/eudralex/index\\_en.htm](http://ec.europa.eu/health/documents/eudralex/index_en.htm)

<sup>45</sup> REGULATION (EC) No 648/2004 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 31 March 2004 on detergents

The international program on chemical safety (IPCS) developed concepts for the assessment of mixtures regarding human health. Concepts are mainly based on the so called toxicity equivalent factor approach (TEF-approach). This approach is mainly used to determine the toxicity of mixtures of dioxins and related chemicals but can also be applied to other mixtures. The TEF is set in relation to the toxicity of 2,3,7,8 tetrachlorodibenzodioxine and calculated for humans, mammals, birds and fish.

A general framework for the assessment of mixture toxicity has been published by the IPCS in 2009<sup>46</sup>, which defines relevant terms and sets out a tiered approach to risk assessment. Concentration Addition is suggested as standard approach to predict hazards of mixtures.

#### **4.4.2 Organization for economic co-operation and development**

The OECD has not yet provided any detailed concepts for assessing the toxicity of mixtures. A detailed workshop report has been published on risk assessment of combined exposures to multiple chemicals<sup>47</sup>.

#### **4.4.3 USA**

According to the EU report on mixture toxicity<sup>48</sup>, the US employ the most advanced approaches to mixture risk assessment and regulation; however these are mostly limited to human health. Two areas are described in relation to the environment: the assessment of contaminated sites and the assessment of pesticides residues in food for substances with common modes of action.

In an UBA report<sup>49</sup> three approaches for the assessment of mixture toxicity under the US regulatory system are identified: non-standardized approaches to plant protection products, an approach called "toxicity identification evaluation" and whole effluent toxicity assessment.

According to the UBA report, in the US system for plant protection products information from testing is preferred over modelled data. Nevertheless, Concentration Addition may be applied for the individual components: the LD50 of a mixture is determined by adding the quotients of the LD50 values and the concentrations of the individual substances in the mixture.

In the so called toxicity identification evaluation (TIE) for water contaminants (complex mixtures) the assessment is based on additivity of effects. No details of the respective methodology could be identified in the UBA report.

The whole effluent toxicity assessment consists of specific and tiered toxicity testing of complex effluent mixtures. It aims at determining the overall toxicity of

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<sup>46</sup> The document is not to be cited or quoted as it is still in a draft status; available at: <http://www.who.int/ipcs/methods/harmonization/areas/combinedexposure.pdf>

<sup>47</sup> OECD: Workshop report Risk Assessment of Combined Exposures to Multiple Chemicals, Series on Testing & Assessment No. 140, February 2011, Paris, France.

<sup>48</sup> The School of Pharmacy University of London (ULSOP): State of the Art Report on Mixture Toxicity Final Report, London, December 2009.

<sup>49</sup> Bericht über den Stand der Ergebnisse zum Arbeitspaket 2.1 'Grundlegende Fragestellungen' im Rahmen des UBA-Forschungs- und Entwicklungsvorhabens „Ökotoxische Kombinationswirkungen von Stoffgemischen“ FKZ 3709 65 404

effluents as well as the contributions of individual substances. This testing approach is discussed and used in different contexts.

In summary, in the US system of assessing toxicities of mixtures either testing is applied or information from the components of a substance are used based on the Concentration Addition model.

#### 4.5 Summary on approaches to assess mixture toxicity

In the current EU regulatory context mixture toxicity is so far only considered to some extent in the authorisation process for plant protection products and biocide formulations. Here, methods are based on the concept of Concentration Addition.

There is evidence that the currently applied substance based approaches for a risk assessment (under REACH) might lead to an underestimation of the actual risks from chemicals in the environment.

Although research is on-going and there are differences in the interpretation of approaches and their applicability, there seems to be a broad agreement on the following:

- The overall **toxicity of a mixture** is a result of the joint action of the individual components and may exceed the toxicity of the most toxic ingredient.
- The use and emission of single substances and mixtures will result in **combined exposures to chemicals in environmental compartments**.
- In regulatory contexts requiring the assessment of mixture toxicity, the model of Concentration Addition is most widely used.

Single substance data, which is needed for predictions of mixture toxicity with the concept of Concentration Addition (or Independent Action) should be available for registered substances in ECHA's data base (LC/ECx values).

#### 4.6 Mixture toxicity in the context of REACH

##### 4.6.1 Legal obligations

REACH attributes the responsibility for safe use of a substance on its own, in a mixture or in an article to the entire supply chain. The task of the identification of operational conditions (OCs) and risk management measures (RMMs) is part of the chemical safety assessment (CSA) of the registrant. The responsibility for the CSA lies with the substance manufacturer/importer.

The formulator is responsible to ensure that no risks occur from the formulation and use of the substances contained in his mixture. He is also responsible for forwarding information on OCs and RMMs for (substances in) the mixture. REACH does not require any risk assessment of the mixture itself, including the

assessment of joint action of the mixture's components, neither by the registrant nor by the formulator. Hence, it is always a voluntary action, if a formulators assesses:

- 1) if interactions between the mixture components may occur;
- 2) how mixture toxicity determines the selection of risk management measures;
- 3) whether joint action of substances in the mixture should be considered in providing information to DUs.

#### **4.6.2 Added value of mixture toxicity assessments to information consolidation**

The aim of consolidating information on mixtures<sup>50</sup> is to provide downstream users (DUs) with all necessary information on the conditions of use (OCs and RMMs) to safely use the (substances in the) mixture in an understandable and concise form.

An assessment of mixture toxicity would provide an "added value" to the consolidation of information received from the supplier if it contributes to a modification of OCs and RMMs, either by

- ensuring adequate control of risk that would not be ensured if the focus was on single substance information or
- focusing the needed RMMs by contributing to the identification of major drivers of risk and related exposure routes.

Vice versa, a mixture toxicity assessment is superfluous if no combined exposures<sup>51</sup> of the environment occur or if the assessment does not contribute to the selection of the "best" conditions of use (CoU). Whereas the former case could be predicted from the emission and fate behaviour of substances, the latter can only be determined after the assessment is concluded.

Cases where combined exposures could occur should be limited to those situations, for which actors under REACH are responsible: Registrants are responsible for assessing risks which could occur from the identified uses and the amounts of the substance they register. In analogy, formulators are responsible for risks resulting from their own use (formulation of mixtures) and the use of their mixtures by their downstream users. Neither registrants nor formulators are obliged to consider effects from the accumulation of substances in the environment<sup>52</sup> or from joint actions of "their" substances with the same or other substances manufactured or used by other actors which are not their DUs.

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<sup>50</sup> If a formulator forwards ESs of single substances to the DU, it is not likely that an assessment of mixture toxicity would be performed. Therefore in the context of mixture toxicity it is always assumed that the formulator consolidates information for his customers.

<sup>51</sup> Combined exposure in this context means the simultaneous presence of substances contained in a mixture in an environmental compartment.

<sup>52</sup> In the context of substance evaluation, registrants and downstream users may be made responsible for accumulation or joint actions, but this is not the "standard case".

Once emitted to the environment, the substances of a mixture partition to the different compartments, depending on their physico-chemical properties. Since the origin of substances contributing to combined exposures of the environment cannot be clearly attributed to an emission from a definite source or allocated to a particular actor, only acute combined exposures (before degradation and partitioning takes place) should be regarded as relevant for the assessment of mixture toxicity. Consequently, no combined exposures at regional level or via the food chain should be included into the CSA procedures of a registrant or the consolidation of information by formulators under REACH.

At local scale, combined exposures could occur in those compartments into which the substances in the mixture are directly emitted. According to the ECHA IR/CSA guidance, at local scale mixing and adsorption to organic matter are taken into account in the CSA. Consequently, the following compartments should be taken into account in checking, whether combined exposures could occur at local scale:

- Freshwater (saltwater, if direct emission)
- STP
- Air

Sediments could be included in the assessment as well, as they are subject to combined exposures at the point of discharge of a mixture with wastewater. Combined exposures to soil should only be considered, if there is a direct emission to (non-industrial) soils, as deposition via the air would normally not result in relevant combined exposures to the substances originally contained in the mixture (very high dilution, origin not traceable).

If combined exposures in the environment are possible, the formulator by consolidating information from the suppliers would ensure that the emissions of the relevant substances are controlled with appropriate measures. A mixture toxicity assessment could result in that the CoUs recommended by the suppliers are not sufficient to adequately control the risks from combined exposures and resulting joint action of substances. Hence, the mixture toxicity assessment would highlight the need for limiting emissions on the relevant emission pathways:

- If several substances reach the same compartment via the same emission pathway it should be ensured that the recommended emission controls are effective for all of the relevant substances.
- If several substances reach the same compartment via different emission pathways it should be ensured that risk management is recommended for all relevant emission pathways. Priorities could be set based on the emitted amounts per emission pathway and/or the persistence of the substances in the compartment which is exposed.
- If adequate control is checked based on the toxicity of the mixture in the environment, the RCRs of all substances contributing to the joint action should be added up.

In summary, the assessment of mixture toxicity (hazard assessment) or of risk characterization ratios that take joint action of substance from combined exposures into account provide a more specific view on the question of whether



or not the risks from the use of a mixture are adequately controlled. However, this information does not allow deducing the emission pathways of substances from the mixtures or the effects of RMMs on the exposure levels; i.e. the formulator gets a better picture on the level of risk but is not supported in his decision on how to best reduce it by recommending appropriate conditions of use. An indication of the risk level and the contribution of the different components in the mixture to that risk may support the prioritization of RMMs or indicate that the efficiency of RMMs recommended by the suppliers should be adapted.

#### **4.7 Conclusions on mixture toxicity assessments for the consolidation of information by the formulator**

The concept of Concentration Addition is the most common approach for the prediction of mixture toxicity if single substance data is available. Testing of mixtures as a whole is well accepted as well (except for biodegradability and bioaccumulation) if the mixture as such is available.

The method of DPD<sup>+</sup>, which is introduced in detail in Chapter 6, ranks the relevance of substances in a mixture with regard to the degree by which they determine the overall risk of a mixture. The substance(s), which is (are) contributing most to the overall toxicity of the mixture is (are) called lead substance (LS).

DPD<sup>+</sup> is a method to consolidate information on the safe use of substances to be forwarded in the supply chain. This process normally does not involve any risk assessments, neither for substances as such nor for the mixture as a whole. Consequently the developers of DPD<sup>+</sup> did not intend to include mixture toxicity assessment and related considerations in the method and therefore the method is also not useful for this purpose. Nevertheless, DPD<sup>+</sup> to some degree allows for a consideration of joint action of two substances. This is the case if the lead substance indicators (LSI) of two substances differ only by 10%. Then both substances should be considered as a lead substance (c.f. Chapter 6). The "10-percent-rule" cannot be related to the classification rules for preparations and no justification is provided in the guidance for this approach.

A consequent implementation of mixture toxicity in the consolidation of information (based on the model of Concentration Addition) would mean to select all mixture components which are hazardous to the aquatic environment as "lead substance". As the core idea of DPD<sup>+</sup> is to prioritize substances to simplify information consolidation, this contradicts the core of the method.

Mixture toxicity aspects could also be included in DPD<sup>+</sup> as "final check" of whether the consolidated information ensures adequate control of risks, even if joint action occurs. This would require the derivation of RCRs for the mixtures, e.g. as carried out in the assessment of biocide products (c.f. Section 4.3.6) for all compartments, where combined exposures could occur (c.f. Section 4.6.2).

The derivation of RCRs for the mixtures is likely to be resource intensive and potentially not possible due to the lack of data and/or the lack of abilities of the formulator to request that information from his supplier(s) (c.f. Section 4.7).

In the context of consolidating information for mixtures, the information on the toxicity of the mixture is however not very helpful, because the mixtures are normally not directly applied to the environment but used in industrial processes, by professional users and / or by consumers.

The added value of a mixture toxicity assessment by the formulator could be a check, if the OCs and RMMs recommended for the mixture after consolidation actually ensure safe use - not only for the individual components but also in situations where joint action could occur. To carry out such check, the RCRs<sup>53</sup> of a mixture in the different environmental compartments are needed, rather than the toxicity of the mixture.

Under biocides and plant protection products legislation, RCRs for mixtures are the sums of the PEC/PNEC ratios for all components contributing to an effect. Hence, formulators would need for each substance

- the PNECs or respective ecotoxicity data to derive the PNECs
- the PECs in the compartments where combined exposure occurs

The PNEC values may in many cases not be available, e.g. because the substance is registered only in the lowest tonnage band (no CSA conducted and / or only two tests performed). It is also likely that the formulator does not have access to the exposure levels, e.g. because they have never been calculated (no CSA conducted) or because they have been "lost" in the communication chain (mixtures used as input materials). Whereas PNECs are published in the ECHA data base, PECs can only be obtained by the formulator by requesting them from the supplier or by generating them through an exposure assessment. The latter would require data collection also on the PC-properties of substances in order to use e.g. EUSES.

In general it can be expected that the high efforts in data collection and data processing required for an assessment of mixture toxicity are disproportionate to the information outcome related to the safe use of a mixture.

Consequently, it is not suggested to include mixture toxicity assessment in the selection of lead substances in accordance with the DPD<sup>+</sup>-method (other than the "10%-rule") or any alternative approach for the consolidation of information on mixtures. The question may be reviewed once the standard practice on environmental safety assessment and forwarding respective information with mixtures is in place and has become routine for all actors in the supply chain.

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<sup>53</sup> The risk characterization ratio for the mixture is the sum of the individual RCRs of all components of the mixture, as e.g. defined for the assessment of biocide products.

## 5 METHODS ON CONSOLIDATING INFORMATION ACCORDING TO REACH

The consolidation of information on the conditions of use (CoU) of mixtures is not an entirely new task for formulators because information on risk management measures (RMMs) in safety data sheets (SDS) of substances had to be used to compile SDSs for mixtures. However, under REACH, more detailed information is to be processed: the operational conditions (OCs) and risk management measures (RMMs) may be described more precisely; and quantitative information on efficiencies of emission and exposure reduction are to be combined.

The ECHA guidance for downstream users (DU) has been developed to provide respective support to formulators. It was published in May 2008 and therefore should be regarded as “theoretical”, as no practical experiences from work with REACH information could be integrated. In the following two chapters, the related content of the guidance document<sup>54</sup> is briefly introduced.

### 5.1 Information on preparations to be delivered by formulators

Chapter 14 of the ECHA guidance, “Information on preparations to be delivered by formulators” describes the legal obligations and outlines a workflow to structure and support the collection, processing and use of information on CoU in the development of eSDSs and other information for mixtures. The formulators’ legal obligations are described in Section 2 of this report.

The workflow and approach proposed in the DU guidance are characterized by the following main elements:

- A consolidation of information is discussed for mixtures, for which an eSDS has to be provided or which requires information for consumers to be displayed on a label;
- Substances which are contained in mixtures below the consideration thresholds defined in REACH Article 14(2) may be disregarded;
- The derivation of CoUs is based on the information in exposure scenarios (ESs) relating to the specific use of the mixture but information from eSDSs is to be used in addition;
- If several substances require risk management for a specific exposure route, the so called critical component approach (c.f. next paragraph) should be applied to identify the RMMs for the mixture;

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<sup>54</sup> ECHA guidance for downstream users, Helsinki, January 2008; available at [http://guidance.echa.europa.eu/docs/guidance\\_document/du\\_en.pdf?vers=29\\_01\\_08](http://guidance.echa.europa.eu/docs/guidance_document/du_en.pdf?vers=29_01_08)

- Concentration Addition should be applied in case more than one substance contribute to a risk; this should be assumed according to the rules of the dangerous preparations directive (DPD) regarding which effects of a substances are additive and which aren't. In these cases, RMMs should be determined based on the added risk characterization ratios (RCRs)<sup>55</sup>;
- A check is recommended at the end of the work process to ensure that the finally recommended OCs and RMMs are not conflicting and appropriate for the use.

The critical component approach (CCA) mentioned in the ECHA guidance has never been described in its Appendix 2 and hence, there is no documentation of how it actually works. The DU guidance states on p. 82:

“The critical components are those substances that determine the risk for one or more adverse effects via one or more exposure pathways. To determine whether or not a substance is ‘critical’, a comparison of the substance’s risk potential is necessary, taking into account its hazardousness (DNELs/PNECs, mobility, vapour pressure, water solubility etc.) and its concentration in the preparation. The risk characterization ratios of your suppliers in section 8 of the exposure scenario of the substances, as such and contained in preparations, may also give an indication of which components are critical. The lower the risk characterization ratio, the less critical the substance may be.”

Hence, it is assumed in the ECHA guidance that for each exposure route one component of the mixture determines the level of risk<sup>56</sup>. Furthermore, the DU guidance assumes that if the RMMs for all exposure routes are selected in a way that adequate control of risk is achieved for all risk-determining substances, the risks from the mixture are also adequately controlled. This aspect is discussed further in the context of the analysis of DPD<sup>+</sup> (c.f. Section **Fehler! Verweisquelle konnte nicht gefunden werden.**).

The following table summarises the main elements of the DU guidance regarding the compilation of information for mixtures.

Table 5.1: Method to consolidate information on mixtures (ECHA DU guidance)

| Item              | Compilation of information for mixtures according to the ECHA DU guidance  | Comment   |
|-------------------|--|---|
| Scope             | Any chemical mixture   |   |
| Stated limitation | None   | The approach is not recommended for PBTs/vPvBs, as no risk can be identified.   |
| Main work steps   | <ul style="list-style-type: none"> <li>• Select subst. if <math>C_{mix} &gt; C_{lim}</math></li> <li>• Select relevant ES (relevant = refer to uses) and compile information, also from SDSs</li> <li>• Select OCs</li> <li>• List PNECs and RMMs per exposure route</li> <li>• Consolidate RMMs per exposure route</li> </ul> | Some steps in the workflow, e.g. checking compliance with the own conditions of use, are not in the scope of this project, as they don't concern the consolidation of information. PNECs may not be available for many substances |

<sup>55</sup> This is the same approach as implemented for the risk assessment of biocide products.

<sup>56</sup> With view to the discussion of mixture toxicity this cannot be fully supported by the authors of this report.

| Item  | Compilation of information for mixtures according to the ECHA DU guidance   | Comment   |
|---|---|---|
| Steps to identify CoUs to forward to the customers          | <ul style="list-style-type: none"> <li>If only one substance is relevant per hazard / exposure route, information from supplier may be used directly</li> <li>If more than one substance is relevant for an exposure pathway, the critical component approach (CCA) may be applied.</li> </ul>  | Substances below concentration limits may be disregarded in the assessment.<br>CCA approach is not clearly explained <sup>57</sup> .  |
| End-points / compartments                                   | Compartments: water, STP, sediment, air and soil<br>No specification of effect types(e.g. acute or chronic)<br>Information on mixture should support assessment   | Biota is not mentioned  |
| Substance properties  | Section 9 of the SDS <sup>58</sup> should be considered to determine exposure routes  | It is not specified which information should be used and how  |
| Method to identify and quantify OCs                         | Information sources: Information received from supplier, own knowledge on uses<br>Identification of OCs: No details – information from checking coverage of ES to be used to define OCs<br>Level of detail: examples of information types to be considered are provided in the guidance; e.g. application technique, critical amounts and local environmental conditions<br>Quantification: not specified   | Assumptions for consolidation methods derived from the DU guidance: <ul style="list-style-type: none"> <li>OCs should cover all conditions in the received ESs</li> <li>ESs may be scaled if OCs differ from the defined conditions</li> <li>Level of detail should as a minimum correspond to information in ERC</li> </ul>  |
| Method to identify and quantify RMMs                        | Information sources: Information received from supplier, compliance check of ESs, SDSs<br>Selection of RMMs: from ES, SDS (section 7 and 8) and compliance check<br>Level of detail: not specified<br>Quantification: not specified<br>Procedure: <ul style="list-style-type: none"> <li>List of RMMs per exposure route</li> <li>If only 1 substance is relevant– copying of RMM from supplier.</li> <li>If more than 1 ES is relevant – compilation of all measures, removal of duplicates; application of critical component approach; selection of RMM from ES of risk determining substance(s); addition of risk if more than 1</li> </ul> | Assumptions for consolidation methods derived from the DU guidance: <ul style="list-style-type: none"> <li>RMMs must cover efficiencies from all RMMs in received ESs (and SDS, if provided)</li> <li>ESs may be scaled to adapt information if RMMs differ</li> <li>Level of detail should include as a minimum the emission pathway</li> <li>Quantification is needed if RMM is obligatory</li> </ul> |
| Checking Conditions of Use (CoU) to ensure control of risks | <ul style="list-style-type: none"> <li>1 critical component (CC) per exposure route: check consistency with other measures</li> <li>&gt; 1 CC per exposure route: add RCRs of these CCs, check if sum of RCRs &lt; 1</li> <li>Scaling possible if different RMM efficiencies are provided</li> </ul>  | Critical component approach is not described.   |
| Communication   | Provision of information in a form that is appropriate to the customers. PNECs for all substances above C <sub>lim</sub> and RCRs should be communicated (not an obligation / requirement)  |   |

## 5.2 Downstream user CSR for mixtures

Section 7.6 of the ECHA guidance for downstream users outlines a proposal for developing a chemical safety report (CSR) for mixtures<sup>59</sup>. The core element to identify the CoUs for a mixture according to the DU guidance is the critical component approach which, as described above, is not defined in any of the ECHA guidance documents up to now. Since a CSR for a mixture may involve similar considerations and methods to derive CoUs for the mixture, the work

<sup>57</sup>There is no information in the available guidance on how to determine a critical component (ECHA DU guidance Section 7 and Section 14, ECHA CSA/CSR guidance and the final report of RIP 3.22 on preparations were checked).

<sup>58</sup> Page 112 of the ECHA DU guidance.

<sup>59</sup> Whether or not a DU CSR for mixtures is possible under REACH is not discussed here.

steps characterizing the approach of the DU guidance are described in the following table.

Table 52: Chemical safety assessment for mixtures according to the ECHA DU guidance

| Item                                    | Characteristics of the CSA for mixtures according to the DU guidance  | Comment   |
|---|---|---|
| Scope                                   | Any chemical mixture  | Assumption in the guidance: if the assessment covers the critical components CCs in the mixture, all substances in the mixture are covered.   |
| Stated limitation                       | None  | No limitations regarding PBTs/vPvBs are made, which is critical, because no RCRs can be derived for such substances and hence an identification of CCs based on RCRs may be misleading.   |
| Main work steps                         | <ul style="list-style-type: none"> <li>• Select only substances above <math>C_{lim}</math></li> <li>• Identify critical components (CC)</li> <li>• Check additivity and consider matrix effects</li> <li>• List critical components</li> <li>• Develop ES for preparation</li> <li>• Calculate RCRs for CCs</li> <li>• Check coverage of all substances by CCs</li> <li>• Compile CSR and ES for SDS</li> </ul> | <p>Disregarding substances below the consideration limits contradicts the overall CSA approach of the DU guidance, because it is assumed that concentration addition should be considered in the identification of critical components.</p> <p>It is not clearly spelled out what "check additivity" means. Assumption in the project: if additive effects occur, all contributing substances are "critical components"</p> |
| Method to identify risk parameters      | <p>Critical component approach, considering PNECs, PC-properties and conc. in mixtures. Communicated RCRs can give indications.</p> <p>Not registered substances or substances without ES must be taken into account. Additivity rules of the Dangerous Preparations Directive are to be applied.</p> <p>Matrix effects changing the mobility of substances in preparations should be taken into account</p>    | Concrete method is missing.   |
| End-points / compartments               | As for substance CSA  |   |
| Substance properties                    | Any properties relevant for the assessment, as for substance CSA  | Section 7.8 on DU CSR for substances mentions: vapour pressure, molecular weight, log $K_{ow}$ , water solubility, degradability  |
| Method to identify and quantify OCs     | For each pathway / endpoint, the OCs are selected that ensure adequate control for the critical component(s)  |   |
| Method to identify and quantify RMMs    | For each pathway / endpoint, the RMMs are selected that ensure adequate control for the critical component(s)   |   |
| Checking CoU to ensure adequate control | <p>RCRs &lt; 1 for each end-point and relevant CC</p> <p>Coverage of other substances by CCs, not specified how</p>   |   |
| Communication                           | As for substances, no specific information  |   |

### 5.3 Conclusions on the ECHA DU guidance

The process of identifying conditions of use – operational conditions and risk management measures – based on the information received with substances or mixtures is unique to the REACH regulation. Hence, apart from the ECHA DU guidance, no alternative methods and approaches could be identified. Both sections of the ECHA guidance dealing with information on conditions of use for mixtures contain a prioritization step: the most critical component of a mixture is selected and the information in the respective ES forms the basis of the information to be forwarded. The critical component approach is not described in the ECHA guidance and can therefore not be discussed here. A critical

reflection on prioritisation of substances regarding their relevance for the overall risks and the selection of conditions of use is included in the analysis of DPD<sup>+</sup> and the conclusions from this project (c.f. Sections 9, 10 and 0).

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## 6 DESCRIPTION OF DPD<sup>+</sup>

### 6.1 Introduction

The method DPD<sup>+</sup> was developed by CEFIC<sup>60</sup> based on a first proposal by two of its sector associations (ESIG and FEICA), which was discussed in a workshop in May 2008 between industry, the European Commission and ECHA. CEFIC states that DPD<sup>+</sup> is one way of implementing the workflow on preparing information for mixtures outlined in ECHA's downstream user guidance (c.f. Section 5.1).

The method's name DPD<sup>+</sup> is derived from the abbreviation of the Dangerous Preparations Directive (DPD), indicating that it is based on the principles of classification and labelling and that there is more and different information to process than for classification by adding the "+".

DPD<sup>+</sup> covers information compilation regarding human health and the environment. In this project, only the environmental aspects are analysed and discussed.

*Note: DPD<sup>+</sup> has been interpreted and used by different actors, e.g. the VCI based its guidance document on DPD<sup>+</sup>, it is programmed into the ES modifier tool and used by some big companies. Any of the users may interpret the methodology differently and consider specific aspects in addition. In particular the way the "checking of consistency" is performed determines the quality of the output of using DPD<sup>+</sup>. Because it is not possible to evaluate all of its potentially "modified", the interpretation of DPD<sup>+</sup> in this report is strictly limited to the description of the method by CEFIC.*

### 6.2 Applicability and limitations of DPD<sup>+</sup> (with focus on the environment)

In principle, DPD<sup>+</sup> can be used to compile information on the conditions of use (CoU) for any mixture. However, CEFIC limits its applicability by excluding mixtures containing

- substances with CMR classification of category 1 & 2,
- substances with PBT/vPvB properties and
- endocrine disrupters.

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<sup>60</sup> CEFIC: REACH: Exposure scenarios for preparations - Methodology for the identification of substances that represent the dominant risks to human health and/or the environment and the drivers for risk management measures, June 2009; [http://www.cefic.org/Documents/IndustrySupport/ES\\_for-preparations-DPD+methodology.pdf](http://www.cefic.org/Documents/IndustrySupport/ES_for-preparations-DPD+methodology.pdf)



### 6.3 Work process of DPD<sup>+</sup>

The workflow in the CEFIC guidance (Figure 1)<sup>61</sup> integrates DPD<sup>+</sup> in the overall process of compiling and providing information for mixtures. It corresponds to the workflow for preparing information for mixtures of the ECHA DU guidance (c.f. Section 5.1). It includes three main steps:

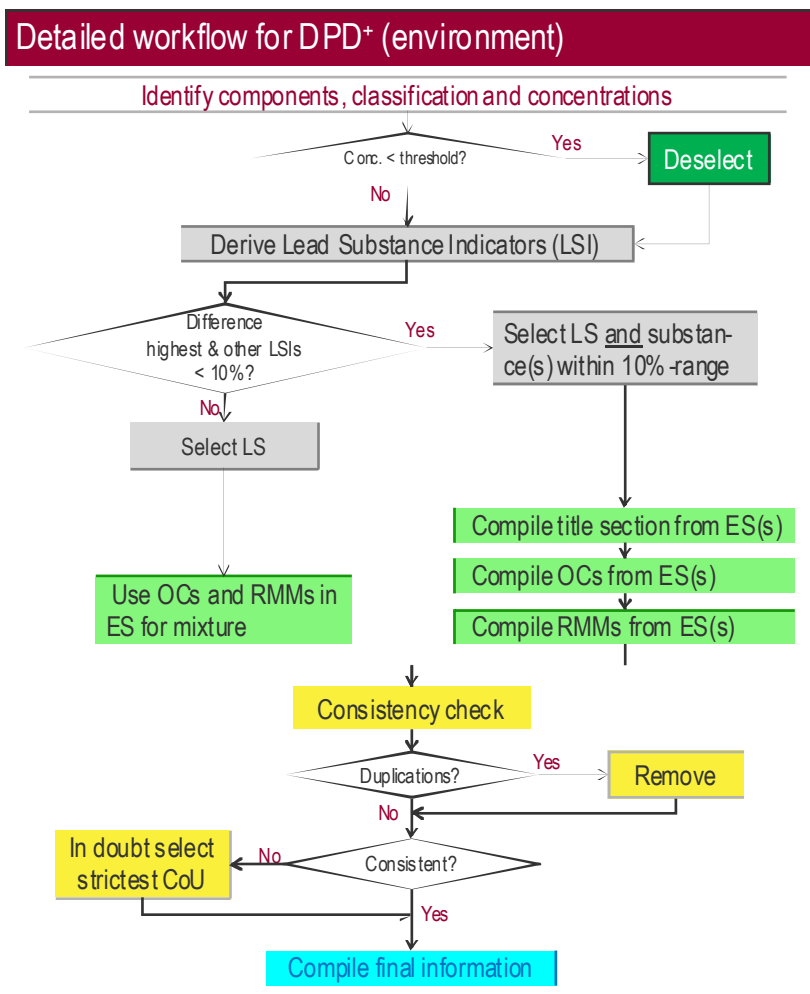
- 1) compilation of information on the mixtures' components (classification, concentration in the mixture<sup>62</sup>),
- 2) selection of lead substances (LS) and
- 3) compilation of information on CoUs for the mixture.

In the following, DPD<sup>+</sup> is described only with regard to environmental aspects. The workflow is illustrated in the following figure.

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<sup>61</sup> The workflow includes a check of whether the received information (ES) is applicable to the specific concentration of the substance in the mixture produced by the formulator (second diamond: "ES applies to dilution?") and may be followed by a scaling step, if that is not the case.

<sup>62</sup> For the selection of CoUs related to human exposures, also the volatility of substances is relevant; since the project only concerns the environmental aspects, this is not mentioned here.

Figure 2: Workflow for using DPD<sup>+</sup> (CEFIC guidance, modified by Ökopoi)

### 6.3.1 Compilation of information Step 1

For the first step, information on the components of the produced mixture should be collected. CEFIC provides general rules for evaluating information in exposure scenarios (ES) but does not explicitly mention safety data sheets (SDSs) as information source to include in the consolidation work. It is therefore anticipated in this project that only substances which have an ES are considered according to DPD<sup>+</sup>.

Information to be compiled (for substances that have an exposure scenario) are the classification and the concentration in the (produced) mixture. If mixtures are used as input material the formulator should use the upper value of the concentration range to derive the concentration in his own mixture.

### 6.3.2 Identification of lead substances for the environment (step 2)

Lead substances are identified for 5 different exposure routes (human health: inhalation, dermal, eyes and ingestion; environment: aquatic environment).

The identification of the LS(s) for the environment is based on a substance's environmental classification, its concentration in the mixture ( $Conc_{mix}$ ) and the respective concentration thresholds for classification ( $Conc_{lim}$ ); the latter are provided in the CEFIC guidance. For each substance a lead substance indicator (LSI) is derived based on the following table.

Table 6.1: Information on substances for using DPD+ (shaded cells to be filled by the formulator)

| Substance    | R-phrase | Limit conc. ( $Conc_{lim}$ )   | Actual conc. ( $Conc_{mix}$ ) | LSI according to equation:            |
|--------------|----------|--|-------------------------------|---------------------------------------|
|              | R 53     | 25 %   |                               | $LSI = Conc_{mix} / Conc_{lim}$       |
|              | R 52/53  |  |                               | $LSI = Conc_{mix} / Conc_{lim}$       |
|              | R 51/53  | 2.5 %  |                               | $LSI = Conc_{mix} / Conc_{lim}$       |
|              | R 50/53  | 0.25 %   |                               | $LSI = Conc_{mix} / Conc_{lim}$       |
|              | R 50     |  |                               | $LSI = Conc_{mix} / (3 * Conc_{lim})$ |
| R50 & R50/53 |          | Specific concentration limits may have been introduced or may have to be derived according to Table 1b or 2 of Directive 1999/45/EC. |                               |                                       |

The  $Conc_{lim}$  values correspond to the lowest concentration thresholds triggering a classification according to Directive 1999/45/EC. An exception is the R50 which cannot trigger classification in a lower environmental category but is grouped together with R50/53<sup>63</sup>.

The LSIs of all substances are compared. The highest LSI determines the lead substance. Substances with an LSI within 10% of the LSI of the lead substance should be identified as additional lead substance. CEFIC provides no reasoning for the value of 10%. For these lead substances the ESs are selected to derive the CoUs for the mixture.

### 6.3.3 Compilation of CoUs relevant for the environment (step 3)

The work process described in the CEFIC guidance consists of the following steps (concerning the environment):

- Checking that for all uses of the mixture an ES is available for the lead substance(s). Ensuring that use descriptors, dilution in the mixture and risk management measures (RMMs) in the relevant ESs cover the actual use. Inclusion of information in the ES for the mixture:
  - title section of the ES format<sup>64</sup> and use descriptors
  - product characteristics
  - intended uses
- Based on the ES of the identified LS(s)

<sup>63</sup> The concentration limit for substances classified with R50 is multiplied by the factor 3 to take account of their ready degradability.

<sup>64</sup> The references in the CEFIC guidance relate to an older version of the ES format; in the updated ES format, the sections have been reorganized and are not numbered anymore. No direct references to the ES – format are included here.

- Inclusion of all information on operational conditions (OCs) and RMMs related to the environment (exposure route water)
- Review of information and editing to remove replications and ensure consistency<sup>65</sup> with individual substance ES. In case of differences, the highest or most demanding OC and/or RMM must be selected.

No details are provided in the CEFIC guidance on how to conduct the above steps. For example it is not explained what “ensure consistency” actually means and what type of information from which substances should be taken into account in this step. This makes it difficult to determine the output of using DPD as it is not standardized and depends on the interpretation of the formulator on how to perform the check.

The examples in the CEFIC guidance as well as in the VCI guidance also do not illustrate how conditions of use are selected in detail and which rules or assumptions inform that process.

#### **6.4 VCI guidance implementing DPD<sup>+</sup>**

On the basis DPD<sup>+</sup> VCI elaborated a guidance document on the exposure assessment and communication in the supply chain especially for mixtures under REACH<sup>66</sup>. As by CEFIC, the consolidation of information is described and limited to mixtures not containing SVHCs<sup>67</sup>. The process of the selection of lead substances is described in more detail in the VCI guidance compared to the CEFIC guidance and additional steps (control steps) are introduced to ensure the quality of SDSs and ESs.

The control steps relate to answering two questions:

- 1) Are the OCs and RMMs selected for the lead substances also sufficient for the other substances in the mixtures?
- 2) Are the risks from substances with dangerous properties that are not reflected in the classification adequately controlled by the selected OCs and RMMs?

#### **6.5 General challenges for consolidating information for mixtures**

The use of mixtures as input materials may cause several challenges to formulators that relate to the loss of information along the communication chain. Neither the CEFIC guidance nor the ECHA guidance for downstream users

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<sup>65</sup> It is not explained in detail what “ensure consistency” actually means and what type of information from which substances should be taken into account in this step. This makes it difficult to determine the output of using the DPD<sup>+</sup>-method as it is not standardized and depends on the interpretation of the formulator on how to perform the check. This is analysed and discussed in more detail in the exemplification.

<sup>66</sup> REACH Practical Guide on Exposure Assessment and communication in the supply chains, Part III: Mixtures under REACH, March 2010 <https://www.vci.de/Themen/Chemikaliensicherheit/REACH/Seiten/REACH-Praxisfuehrer.aspx#>

<sup>67</sup> The guidance contains a separate chapter outlining some ideas on how to proceed if a mixture contains SVHC.

provide concrete advice on how to overcome these challenges. These may include:

- Lack of information on the actual substance concentrations in mixtures  
*CEFIC and the DU guidance recommend using the upper end of concentration ranges.*
- Lack of information on the content of environmentally relevant substances which don't have to be indicated on the list of ingredients<sup>68</sup>  
*This is not explicitly mentioned by CEFIC or the ECHA guidance.*
- Information on hazards other than indicated by the classification is normally not communicated for the components in the mixture but only the mixture itself.  
*As CEFIC interprets the obligation to forward information as linked to a classification, it works with R-phrases and therefore this issue doesn't occur in the DPD<sup>+</sup>-method. This issue is also only briefly mentioned in the DU guidance.*
- Information on OCs and RMMs for mixtures may be aggregated for all contained substances classified for the environment  
*CEFIC and the DU guidance do not mention this potential problem<sup>69</sup>.*

Two more issues are observed in the DPD<sup>+</sup>-method which are included in a different way in the DU guidance:

- CEFIC does not explicitly mention the use of information in SDSs or Article 32 information for substances or mixtures used as input materials. It is understood that DPD<sup>+</sup> suggests basing the information forwarded with mixtures only on ESs received from suppliers.  
*In the DU guidance the use of any information is implied*
- If no SDS is required, no further action is indicated in CEFIC's workflow, however; if information to consumers or Article 32 information on RMMs is to be prepared, a consolidation step or communication of information may be necessary<sup>70</sup>.  
*This is not explained in the text and the workflow may be misleading.*

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<sup>68</sup> The limitation of the method to the aquatic compartment and the possibilities of overlooking risks to the sewage treatment plant, sediments etc. are discussed in detail in the analysis of the method.

<sup>69</sup> The issue was discussed at EU level in the context of the interpretation of which information should be forwarded by formulators to formulators and the solution was that the ESs of individual substances should be forwarded in particular for mixtures used to make mixtures.

<sup>70</sup> The requirement to forward information only refers to cases where an SDS is prepared; hence explicitly not for consumer products. The DU guidance separates consumer mixtures from other chemical products only at the very last step of the workflow on consolidating information.

## 7 ASSESSMENT OF DPD<sup>+</sup> - SELECTION OF LEAD SUBSTANCES

In the following the detailed assessment of the selection of lead substances (LS) according to DPD<sup>+</sup> are presented. According to the aims of the project, the analysis focuses on identifying which potential risks of a substance could be overlooked by DPD<sup>+</sup>. The analysis consists of

- a review of the classification system. As DPD<sup>+</sup> bases on the classification, risks overlooked by classification would also not be considered in the selection of lead substances;
- a review of substance properties (mobility, persistence and bioaccumulation and (eco)toxicity) with regard to how they could influence risks from substances. As DPD<sup>+</sup> does not include this information in the selection of lead substances, risks may be overestimated or underestimated;

A review of risk assessment reports (RARs) carried out under the Existing Substances Regulation (ESR) is provided in Section 8. That analysis should identify to which extent substances without an environmental classification could pose risks.

The analysis of the method to select LS(s) does not consider which consequences the selection of ("wrong") LS(s) would have on the identification of conditions of use (CoU) of the mixture. This is discussed in Chapter 9.

### 7.1 Classification

The classification rules of the Dangerous Substances Directive (DSD - 67/548/EEC) and the Dangerous Preparations Directive (DPD - 1999/45/EC) as well as the Regulation on Classification and Labelling (CLP-Reg. - (EC) No 1272/2008) were analysed using the legal texts and the pertaining guidance documents.

The classification endpoints and categories / classes and the criteria for assigning them to a substance were described. It was evaluated which environmental hazards that could potentially lead to environmental risks could be overlooked if the classification with R-phrases is used for the selection of lead substances according to DPD<sup>+</sup>.

#### 7.1.1 General rules and comparison of classification systems

The rules for classification and labelling according to DSD (67/548/EEC), DPD (1999/45/EC) and/or the CLP-Reg. ((EC) No 1272-2008) determine whether or not an environmental R-phrase / H-statement is to be assigned to a substance or mixture. Substances are to be classified according to the CLP-Reg. from

01.12.2010 and mixtures from 01.06.2015. Until 01.06.2015 suppliers of mixtures may use both classification systems. Only classified substances are considered in the selection of lead substances according to DPD<sup>†</sup>. For the classification of aquatic toxicity, as a minimum the results of one test on acute aquatic toxicity and information on the degradability and the log K<sub>ow</sub> are needed. This information is available for all registered substances<sup>71</sup>.

In Table 7.1 the criteria for the environmental classification are paraphrased for the DSD/DPD and compared with criteria of the CLP-Reg. for the similar hazard categories / classes. In the two middle columns the consideration thresholds and the concentrations triggering classification of mixtures are quoted.

With the second adaptation to technical progress (2<sup>nd</sup> ATP<sup>72</sup>), additional rules were included allowing the classification of substances for chronic aquatic toxicity based on information from chronic studies: If e.g. NOEC values for algae, daphnia and fish are available, that data should be used for classification together with the degradability of the individual components in the mixture. If no such data exists, the classification is performed according to the above described method and criteria. M-factors apply to the chronic classification as well. The rules for classification based on chronic data are not included in the table as no corresponding possibility exists in the DSD/DPD.

With the same ATP the classification of substance regarding ozone depletion has been introduced to the CLP-Reg. This has been included in Table 7.1, because a corresponding hazard category exists in DSD/DPD.

Table 7.1: Comparison of classification rules according to DSD/DPD and the CLP-Reg.

| Classification <sup>73</sup> | Directive 67/548 <sup>†,74</sup>  | Consider $\geq$ % DSD/CLP <sup>75</sup> | Classify <sup>†</sup> if $\geq$ % DSD/CLP | CLP-Reg.<br>(bold: differences to DSD/DPD)   |
|------------------------------|---|---|---|--|
| Very toxic, acute            | R50<br>LC/EC/IC50 $\leq$ 1 mg/l   | 0.1 / 0.1                               | 25 / 25 <sup>76</sup>                     | Acute Cat 1 (H400)<br>LC/EC50/ErC50 $\leq$ 1 mg/l  |
| Very toxic, chronic          | R50/53<br>LC/EC/IC50 $\leq$ 1 mg/l and<br>not ready degradable or<br>log Kow $\geq$ 3 except BCF $\leq$ 100 | 0.1 / 0.1                               | 0.25 / 0.25 <sup>77</sup>                 | Chronic Cat 1 (H410)<br>LC/EC/ ErC50 $\leq$ 1 mg/l and<br>not degradable or<br>BCF $\leq$ 500 <b>unless</b> Log Kow $\geq$ 4 |
| Toxic chronic                | R51/53<br>1 < LC/EC/IC50 $\leq$ 10 mg/l and<br>not ready degradable or                                      | 0.1 / 1                                 | 2.5 / 2.5                                 | Chronic Cat 2 (H411)<br>1 < LC/EC/ErC50 $\leq$ 10 mg/l and<br>not ready degradable or  |

<sup>71</sup> See REACH Annex VII which sets the minimum requirements for data in the lowest registration tonnage band

<sup>72</sup> Commission Regulation (EU) No 286/2011 of 10 March 2011 amending, for the purposes of its adaptation to technical and scientific progress, Regulation (EC) No 1272/2008 of the European Parliament and of the Council on classification, labelling and packaging of substances and mixtures

<sup>73</sup> Only a summary of the core criteria for the classification of aquatic toxicity and effects to the ozone layer are provided.

<sup>74</sup> For classification, information from acute toxicity tests is sufficient. Results of long term testing can be used to modify an assessment (if NOEC > 1 mg/l certain classifications don't apply).

<sup>75</sup> In either case, more specific concentration thresholds for consideration in classification could be defined and would then have to be followed. According to the CLP regulation, M-factors have to be defined based on the toxicity of a substance. If these exist, the concentration limits have to be adapted accordingly.

<sup>76</sup> The quoted concentrations are the lowest concentration that would trigger a classification of the mixture. R50 can only trigger a classification as R50 (threshold 25%), as all other R-phases are combined with an R53. In the DPD+-method this threshold is set to 0.75%, which is the threshold for R50/53 multiplied by the factor 3. More details on the factor three are given in the section of this report on bioaccumulation and persistence.

<sup>77</sup> The use of M-factors or specific concentration limits could result in lower concentrations triggering classification.

| Classification <sup>73</sup> | Directive 67/548 <sup>74</sup>  | Consider $\geq$ % DSD/CLP <sup>75</sup> | Classify <sup>76</sup> if $\geq$ % DSD/CLP | CLP-Reg. (bold: differences to DSD/DPD)   |
|------------------------------|---|---|--|---|
|                              | log Kow $\geq$ 3 (except BCF $\leq$ 100)  |   |  | BCF $\leq$ 500 unless Log Kow $\geq$ 4<br><b>Not applicable if NOEC &gt; 1 mg/l</b>   |
| Harmful, chronic             | R52/53<br>10 < LC/EC/C $\leq$ 100 mg/l and not ready degradable   | 1 / 1                                   | 25 / 25                                    | Chronic Cat 3 (H412)<br>10 < LC/EC/ErC50 $\leq$ 100 mg/l and not ready degradable <b>or</b><br>BCF $\leq$ 500 unless Log Kow $\geq$ 4<br>Not applicable if NOEC > 1 mg/l  |
| Potentially toxic            | R 52<br>other substances of concern not fulfilling the above criteria.  | 1 / --                                  | 25 / --                                    | Not existing, however partly covered by chronic 4   |
| Long term effects            | R 53<br>Water solubility < 1 mg/l and not ready degradable and log Kow $\geq$ 3 (except BCF $\leq$ 100)<br>Not if NOEC > 1 mg/l | 1 / 1                                   | 25 / 25                                    | Chronic Cat 4 (H413)<br>Safety net concept: substances for which data don't allow classification according to the criteria but that give rise to concern. An example are substances with a water solubility < 1 mg/l and which are not ready degradable <b>or</b> have BCF $\leq$ 500 unless Log Kow $\geq$ 4, except the NOEC > 1 mg/l |
| Dangerous non-aquatic        | R 54/55/56/57/58<br>No specific rules   | 0.1 / 0.1                               | 0.1 / 0.1                                  | Not existing  |
| Dangerous for ozone layer    | R 59<br>Montreal substances and substances giving rise to similar effects based on structural information                       | 0.1 / 0.1                               | 0.1 / 0.1                                  | H420<br>Montreal substances and substances giving rise to similar effects based on structural information   |

### 7.1.2 Concentration thresholds in mixtures

#### Thresholds for identification in the safety data sheet

In both classification systems, thresholds are defined below which substances do not have to be considered in the classification for the environment (consideration thresholds). These consideration thresholds have been agreed as indicating "no concern" or leading to insignificant effects. Substances contained in mixtures below these thresholds do not have to be listed in the safety data sheet (SDS). Hence, formulators using mixtures as input materials will only know of substances in the mixture which are classified and contained in concentrations above the consideration thresholds<sup>78</sup>. All other substances, even if they are classified, cannot be identified by the formulator and hence not considered in any information on his own product.

Consequently, in the project the consideration thresholds of DPD and the CLP-Reg. are regarded as cut-off values also in the context of assessing mixtures under REACH. This means that for consolidating information on mixtures, only substances contained in input materials which are listed in the pertaining SDS under Section 3 have to be considered<sup>79</sup>. This is particularly important with view to the (legal) possibilities of a formulator to obtain information from his supplier in order to make an assessment of the mixture.

<sup>78</sup> In addition, substances with occupational exposure limit values and PBTs/vPvBs may be indicated, if they exceed the related concentration thresholds.

<sup>79</sup> Note that according to DPD\* the formulator only should consider substances that are contained in his mixture (the product he places on the market) in concentrations above the consideration thresholds.



### Thresholds for classification of mixtures

Both frameworks for classification - the DSD / DPD and the CLP-Reg. - define concentration thresholds that trigger the classification of mixtures. If a classified substance is contained in a mixture above the thresholds for classification, also the mixture has to be classified. As shown in Table 7.1 the classification thresholds for the environment are the same in both systems.

The logics of classification are based on grouping substances within ranges of toxicity. Therefore, substances may have the same classification but the degree of toxicity and other properties can vary within a range. For example: a persistent substance with an aquatic toxicity of 1.2 mg/l and a substance with an aquatic toxicity of 9.8 mg/l and a Log Kow of 5 are both classified with R51/53 but their properties are rather different. The consequences with regard to DPD<sup>+</sup> are discussed in Section 0.

### **7.1.3 Bridging principles in the assessment of mixtures**

The bridging principles of the CLP-Reg. apply to the environmental classification, except the rules for aerosols. They can be summarized as follows:

- Dilution: if a mixture is diluted by a substance or mixture with a less hazardous classification, the original classification may be maintained. This could result in a classification that is stricter as if the individual components were assessed using the additivity or summation method of the CLP-Reg.
- Analogous batches: one batch could be classified as another batch of the same production cycle.
- Concentration of mixtures: if a mixture classified with the strictest classification possible is concentrated, the classification is maintained.
- Interpolation within toxicity categories: Three mixtures consist of the same substances in different concentrations. If mixture A and B have the same classification and the concentration of substances in mixture C is between those in mixture A and B, mixture C can be classified as mixtures A and B.
- Similar mixtures: if mixtures contain substances with similar concentrations and similar classifications, the classification can be deduced by comparison and conclusions analogy.
- Table on variability of concentrations: if concentrations are changed within the ranges specified in the respective tables in the CLP-Reg. the classification does not have to be changed.

The bridging principles are only an instrument to facilitate classification. They are not relevant with regard to DPD<sup>+</sup>.

### **7.1.4 Summary of comparison of classification frameworks**

The hazard category "dangerous for the non-aquatic environment" is not included in the CLP-Reg. The respective R-phrases of the DSD have not been assigned to industrial chemicals up to now<sup>80</sup>.

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<sup>80</sup> In contrast to chemicals under the scope of the biocide directive (98/8/EC) which undergo a different testing strategy and to which these R-phrases have been assigned

In the CLP-Reg. no analogous category exists for R52 (potentially toxic); however it is partly included in the hazard category aquatic chronic 4. A few differences exist in the classification criteria of both systems (see last column in Table 7.1). The thresholds for consideration and for classification are the same.

DPD<sup>+</sup> considers all hazard categories related to the aquatic toxicity of substances in its approach. It does not include effects on the ozone layer (R59) or to the non-aquatic environment (R-phrases R54 to R58). The consideration thresholds are used to identify the substances in the produced mixture, which should be included in the identification of lead substances. The classification limits are used as divisors in the equation for identifying the LSI.

The CLP-Reg. includes the possibility to use data from long-term testing for the classification of chronic aquatic toxicity. Hence, different types of data can be used for classification but the logics remain the same. As the basis of DPD<sup>+</sup> currently is the old classification system, this is not further discussed.

The comparison of classification frameworks and the integration of hazard categories and classification rules in DPD<sup>+</sup> are summarized in Table 7.2.

Table 7.2: Summary of findings related to the classification of mixtures and DPD<sup>+</sup>

| Classification endpoint       | DSD/DPD  | CLP-Reg.       | Comparison of systems   | DPD <sup>+</sup> -method                                    |
|-------------------------------|--|----------------|---|---|
| Very toxic, acute             | R 50   | H400           | Same criteria   | Considered in selection of lead substances                  |
| Very toxic, chronic           | R 50/53  | H410           | Log K <sub>ow</sub> and BCF differ  |   |
| Toxic chronic                 | R51/53   | H411           | Log K <sub>ow</sub> and BCF differ; exception in CLP-Reg. if NOEC > 1                         |   |
| Harmful, chronic              | R52/53   | H412           | Possibility to use information on bioaccumulation Log K <sub>ow</sub> / BCF                   |   |
| Potentially toxic             | R 52   | Not existing   |   |   |
| Long term effects             | R 53   | H413           | Log K <sub>ow</sub> and BCF differ; criteria in CLP-Reg. alternatively, in DSD both to be met |   |
| Dangerous non-aquatic         | R 54, 55, 56, 57, 58                                 | Not existing   | Not existing in the CLP-Reg.  | Not considered  |
| Dangerous for ozone layer     | R 59   | H420           | Same criteria   |   |
| Thresholds for consideration  | 0.1 or 1% or, if lower: threshold for classification |                | Same values   | Substances above cut-off in produced mixture are considered |
| Thresholds for classification | 0.25 to 25 or less if M-factor is to be applied      |                | Same values   | Used as divisor for LSI calculation                         |
| Bridging principles           | Basic rules exist                                    | More extensive | Extended in CLP-Reg. and use encouraged   | Not relevant for DPD <sup>+</sup>                           |

### 7.1.5 General conclusions on classification

The classification with R-phrases or H-statements is based on information derived from data on the aquatic toxicity, degradability and bioaccumulation, as well as the water solubility in some cases. For all registered substances information for classification should be available<sup>81</sup>.

<sup>81</sup> According to Annex VII two tests should be performed on the aquatic toxicity: a test on growth inhibition of algae and a test on toxicity to daphnia. The log K<sub>ow</sub> and ready degradability are to be tested as well.

Regarding the DPD<sup>+</sup>-method a change from R-phrases to H-statements of the CLP-regulation would have the following consequences:

- **Different substances may be considered in different classification categories** in the selection of lead substances, due to different classification rules:
  - Substances with log K<sub>ow</sub> between 3 and 4 and/or BCFs between 100 and 500 would be classified according to DSD but not according to the CLP-Reg. (R53 but no chronic aquatic toxicity).
  - Substances with LC/EC/IC50s between 1 and 100 mg/l and NOECs >1 mg/l are not classified under CLP-Reg. but would be classified R51/53 or R52/53 according to the DSD, if persistence or bioaccumulation criteria are fulfilled.
  - More substances would be classified in chronic category 4 than have been classified with R52/R53 according to the DSD because bioaccumulation is an additional criterion.
  - Differences could occur because the connection between the criteria log K<sub>ow</sub> and persistence are different in some hazard categories (and, or, and/or connection).
- Differences would also occur in the **identification of substances in the SDS if contained** in mixtures: Less substances may be identified in the SDS of mixtures (used as input materials) because of a lower consideration threshold of H411 compared to R51/53 (1% / 0.1%) and potentially more would be identified in the classification category chronic 4.

The logics of M-Factors – lowering the classification triggers for substances with LC50 values below 1 mg/l – has been implemented in the DPD by a Commission Directive<sup>82</sup> as adaptation to technical progress in 2006.

*The change of classification frameworks would not cause qualitative changes to DPD<sup>+</sup>.*

#### **7.1.6 Conclusions regarding weaknesses of DPD<sup>+</sup> resulting from its foundation on classification**

DPD<sup>+</sup> is founded on the classification rules of substances and mixtures. Therefore, all risks which are not covered by classification are also not specifically considered in the selection of lead substances.

With the exception of ozone depletion, the classification rules systematically overlook environmental hazards to and via the atmosphere, such as ozone formation and or risks to organisms by inhalation.

Further hazards to the environment which are not reflected by classification are long range transport of substances, the ability of substances to reach (and pollute) the groundwater and hazards to sewage treatment plants, due to toxicity to microorganisms.

<sup>82</sup> COMMISSION DIRECTIVE 2006/8/EC of 23 January 2006 amending, for the purposes of their adaptation to technical progress, Annexes II, III and V to Directive 1999/45/EC of the European Parliament and of the Council concerning the approximation of the laws, regulations and administrative provisions of the Member States relating to the classification, packaging and labelling of dangerous preparations

Although the classification according to DSD foresees R-phrases for the terrestrial environment (R54 to R58), no rules have been developed for assigning them and up to now, no industrial chemicals has been classified respectively. The selection of lead substances according to DPD<sup>+</sup> does also not consider the R-phrases R 54 to R58.

Classification for ozone depletion is indicated by the R59. This R-phrase is not included in the method for selecting LS(s) according to DPD<sup>+</sup>.

All R-phrases and combinations of R-phrases related to the aquatic environment used in the classification according to DSD/DPD are part of DPD<sup>+</sup>, except R52 which has not yet been assigned to any substance<sup>83</sup>. Hence, the aquatic risks are principally covered<sup>84</sup> by DPD<sup>+</sup>.

According to the current interpretation of DPD<sup>+</sup>, all substances which are contained in the mixture produced by the formulator above the consideration thresholds should be taken into account in the selection of lead substances.

If formulators use mixtures as input materials, they receive information on all classified substances contained in the mixture above the consideration thresholds. Only these substances can be considered by the formulator in consolidating information for his product. DPD<sup>+</sup> may exclude some of these substances, as only substances contained in the product above the consideration thresholds should be taken into account.

*Identified weaknesses of DPD<sup>+</sup>: no consideration of R59, terrestrial toxicity and "other" risks to the atmosphere, consideration of substances in the formulated mixture above the consideration thresholds only*

## 7.2 Criteria for scoping exposure assessments (ECHA)

### 7.2.1 Introduction of criteria

The ECHA guidance on information requirements and chemical safety assessment provides criteria to the registrant on when an assessment of environmental safety can be omitted or limited due to an obvious lack of environmental hazards. In the updated version of the guidance<sup>85</sup>, the previously defined clear cut-off criteria have been replaced by several decision trees. A set of different criteria are defined to limit the assessment scope, i.e. certain aspects can be omitted, if the substance meets specific criteria.

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<sup>83</sup> The N-class data base compiling information relevant for the environmental classification of substances and operated by the Swedish Chemicals Inspectorate (<http://apps.kemi.se/nclass/default.asp>) was searched. There may however be self-classified substances with R52.

<sup>84</sup> Weaknesses with regard to the classification system as such and risks to sediments and soils potentially overlooked are discussed in the later sections.

<sup>85</sup> ECHA: Guidance on information requirements and chemical safety assessment; Part B: Hazard Assessment; new chapter B.8 Scope of Exposure Assessment; Version 2.1 (December 2011). ([http://echa.europa.eu/documents/10162/13643/information\\_requirements\\_part\\_b\\_en.pdf](http://echa.europa.eu/documents/10162/13643/information_requirements_part_b_en.pdf)).

Turning around the perspective, substances not meeting the criteria give rise to concern for a specific environmental endpoint. They can therefore be used to characterize substances beyond the legal classification as dangerous, which should be considered in selecting risk management measures (RMMs).

It would be in line with the ECHA guidance to **exclude substances** from the procedure of consolidation of information for mixtures, **if all of the following criteria are met**: The substance is:

- not classified as toxic to reproduction or toxic after long-term or repeated exposure;
- readily degradable;
- has a log Kow < 3 or a BCF < 100 (in case lipid partitioning is the main mechanism of accumulation);
- is assessed as “aquatic toxicity unlikely to occur”<sup>86</sup>;

Substances which are not classified because they are neither persistent nor bioaccumulative but are toxic to aquatic organisms (LC50 above 1 mg/l) could cause environmental risks. As they are not classified they would not be considered by DPD<sup>+</sup>.

Substances which are classified as reprotoxic or toxic after repeated exposure may cause adverse effects if they accumulate in the food chain, which is an environmental endpoint as well. These types of classification are not considered in DPD<sup>+</sup>.

### 7.2.2 Conclusions on safety assessment criteria and DPD<sup>+</sup>

Substances which fulfil all of the criteria defined in the ECHA guidance on the “scope of the exposure assessment” should in general not be regarded as environmentally relevant and therefore not considered in the selection of RMMs. Substances which are not classified but do not fulfil the criteria may contribute to environmental risks and should be considered.

Substances which are not classified are not indicated in the SDSs of mixtures. Therefore, formulators are not able to identify them in their input materials and can also not take them into account in their consolidation work.

It is a voluntary action of the formulator to consider non-classified substances in the consolidation of information for his mixture. No respective legal requirement exists. Non-classified substances must only be considered, if they are SVHCs. This is practically only possible for substances used as such.

*Identified weaknesses of DPD<sup>+</sup>: substances which are not classified as dangerous but may cause environmental risks are not included in the process of selecting lead substances.*

<sup>86</sup> Aquatic toxicity is predicted or it has been shown in testing that the limit doses in OECD testing have been exceeded for any of the trophic levels. Substances are regarded as soluble and are likely to cross biological membranes. No concrete cut-off values exist on when to regard substances as insoluble or unlikely to cross biological membranes.

### 7.3 Substance properties

The information requirements for registration of substances and chemical safety assessment (CSA) were compiled and analysed using the REACH text including its annexes and related ECHA guidance documents. Information for the environmental risk assessment is listed in table form, specifying from which tonnage the information is required and for what it can be used.

#### 7.3.1 Information on mobility

Table 7.3 lists the most relevant types of physico-chemical properties (PC-properties) for environmental safety assessment and specifies from which registration tonnage it is required. Waiving options are not considered. The last column indicates the use of information in environmental risk assessment.

Table 7.3: PC-information for environmental risk assessment

| PC info / mobility            | Tonnage               | Use of information / comments  |
|-------------------------------|-----------------------|--|
| Molecular weight              | any                   | Indicator for permeation of biological membranes   |
| Boiling point                 | > 1 t/a               | Indicator for physical state, state in the environment and volatility, input value to calculate vapour pressure  |
| Relative density              | > 1 t/a               | Indicator for distribution within compartments, gases: indicator behaviour in air, insoluble liquids and solids, determining factor for settling.  |
| Vapour pressure               | > 1 t/a               | Indicator for partitioning, atmospheric concentrations, potential for airborne transport, relevance of photo degradation. Input value to derive partitioning coefficients and select emission factors. Information for test designs. |
| Surface tension <sup>87</sup> | > 1 t/a               | Influence of solubility and availability of hydrophobic materials to organisms, potentially increased penetration of membranes → relevance for mixture toxicity  |
| Water solubility              | > 1 t/a               | Indicator for bioavailability, partitioning and mobility in soil. Information for test design.   |
| Log Kow                       | > 1 t/a               | Indicator for partitioning, sorption, bioavailability, bioaccumulation and ecotoxicity and PBT assessment.   |
| Adsorption / desorption       | > 10 t/a<br>> 100 t/a | Indicator for binding capacity to solid surfaces; elimination with sludge, mobility and accumulation in soil and sediments. Calculation of partitioning coefficients and PNECs from PNEC <sub>water</sub> .                          |
| Dissociation constant         | > 100 t/a             | Relevant to determine accumulation in soil, may determine fate in the environment and bioavailability  |

#### 7.3.2 Summary and conclusions on mobility

##### Chemical safety assessment

The PC properties are important indicators for identifying the emission pathways of substances from processes. As the emission pathways are the actual point of exposure control under REACH, the PC-properties are important for the assessment and information generation for mixtures.

Furthermore, PC-properties influence environmental partitioning, fate and behaviour and hence determine the total exposure and consequently the risk for the different environmental compartments.

<sup>87</sup>Surfactant molecules typically contain both polar (hydrophilic) and non-polar (lipophilic) moieties. Such a chemical structure is used as an initial indicator (alert) of surface-active properties as well as foaming of aqueous solutions.

For emission estimation the vapour pressure (or boiling point), the water solubility and the log  $K_{ow}$  are most important. Also some other parameters should be considered, such as dustiness and stability of the substance in different media.

Table 7.4: Overview of relation between PC-information and emission pathways to the environment

| Emission likely to | Vapour pressure | Water solubility | Log Kow      | Other   |
|--------------------|-----------------|------------------|--------------|---|
| Air                | High            | Low              | Not relevant | Stable in air, no photo degradation, dustiness                          |
| Water              | Low             | High             | Low          | No hydrolysis   |
| Soil               | Low             | High             | High         | Type of mixture and application more relevant than substance properties |

The environmental fate and behaviour is determined by the mobility and some other parameters, like the molecular weight (indicator for ability to cross biological membranes), hydrolysis and photo degradability etc. The tendency to adsorb to organic matter ( $K_{oc}$  derived from adsorption/desorption testing) is a core parameter indicating the partitioning.

Table 7.5 summarizes the main relationships between the different parameters and the tendency of substances to partition to different environmental compartments.

Table 7.5: Overview of relation between PC-information and partitioning in the environment

| Substance partitions to | Vapour pressure | Koc          | Log Kow      | Water solubility | Other   |
|-------------------------|-----------------|--------------|--------------|------------------|---|
| Air                     | High            | Low          | Not relevant | Low              | Half-life in air high<br>No photo degradation |
| Water                   | Low             | Low          | Low          | High             | No hydrolysis                                 |
| Sediment                | Low             | High         | High         | Low              |   |
| Soil                    | Low             | High         | High         | Low              | Ionisable substances                          |
| Biota                   | Low             | Not relevant | High         | Low/high         |   |

The (emission) behaviour of substances may change due to interactions with other substances in the mixtures, e.g. solvents change the solubility of substances in the mixture. These effects are normally not considered by the registrants in their CSA.

Formulators may identify significant influences of substances on each other's PC properties and consequently their emission behaviour. Since formulators know the main components of their products, they may assess respective effects on a case-by-case basis, in particular when mobility of substances is significantly increased. A standardized method is not available and REACH does not contain specific obligations with regard to this.

#### DPD<sup>+</sup>-method

The selection of lead substances does not consider PC-properties, except the log  $K_{ow}$  if that is relevant for the classification. Therefore the relevance of substances in the mixture may not be fully understood with regard to the emission potential and later exposure in the environment.

**Example:**

Table 7.6: Illustration of possible impacts of the PC-properties on the selection of lead substances

| Sub-stance | Classi-fication | Conc limit | Conc mixture | LSI | Solu-bility | Use / day <sup>88</sup> | Waste-water | Amount in wastewater | Conc <sub>water</sub> <sup>89</sup> |
|------------|-----------------|------------|--------------|-----|-------------|-------------------------|-------------|----------------------|-------------------------------------|
| A          | R51/53          | 2.5%       | 35%          | 14  | < 1 mg/l    | 87.5 kg                 | 60 l        | Max. 60 mg           | 0.003 µg/l                          |
| B          | R 51/53         | 2.5%       | 30%          | 12  | 100 mg/l    | 75 kg                   | 60 l        | Max. 6 g             | 0.3 mg/l                            |

In the example it is assumed that a maximum of 60 mg of substance A could be dissolved in the wastewater in accordance with the solubility; substance B dissolves to a much higher degree: 6 g. Assuming no degradation for both substances, resulting concentrations in the local river after the sewage treatment plant (STP) would be 0.003 µg/l (A) and 0.3 mg/l (B). The concentration of substance B would cause higher risks than that of substance A. A similar example could be developed for emissions to air (vapour pressure) or emissions to soil via sludge ( $\log K_{ow}$ ). The example clearly shows that the PC properties should be taken into account in selecting lead substances for the environment.

As a minimum, the parameters vapour pressure, water solubility and  $\log K_{ow}$  should be considered by DPD<sup>+</sup> to reflect the main emission and fate behaviour.

*Identified weaknesses of DPD<sup>+</sup>: no consideration of water solubility, vapour pressure and  $\log K_{ow}$  in the selection of lead substances*

**7.3.3 Degradation and bioaccumulation**

In Table 7.7 types of tests on substance properties determining persistence and bioaccumulation are listed and it is specified for which tonnage ranges they are required. The last column exemplifies how information may be used in environmental risk assessment.

Table 7.7: Compilation of relevant information on fate and behaviour in the environment

| Type of information                                      | Tonnage   | Use of information  |
|--|-----------|---|
| Biodegradation (ready)                                   | > 1 t/    | Screening value for P-criterion, indicator for long-term risks incl. secondary poisoning, classification, waiving criterion   |
| Abiotic degradation (e.g. oxidation, hydrolysis)         | > 10 t/a  | Half-lives in compartments, indicator for long-term risks incl. secondary poisoning   |
| Simulation testing: surface water, soil, sediment        | > 100 t/a | Values to check P-criterion, half-lives in compartments, indicator for long-term risks  |
| Identification of degradation products                   | > 100 t/a | Indicator for long-term effects, relevant for soil toxicity   |
| Aquatic bioaccumulation potential (Log K <sub>ow</sub> ) | > 1 t/a   | Screening value for B-criterion (not applicable if accumulation not driven by lipid partitioning), indicator for long-term risks including secondary poisoning, indicator for fate in the environment |
| Aquatic bioaccumulation potential (BCF fish)             | > 100 t/a | Value to check B-criterion, long-term effects, accumulation in food chain   |

<sup>88</sup> Assumed amount of mixture per day is 200 kg/d<sup>89</sup> Assumed degradation in STP of 30% and dilution with 20.000 m<sup>3</sup>/d



| Type of information                          | Tonnage    | Use of information  |
|--|------------|---|
| Terrestrial bioaccumulation potential (BSAF) | > 1000 t/a | Indicator for accumulation in terrestrial food chain and secondary poisoning, values on plants used for estimating concentrations in food crops |
| Results of a PBT/vPvB assessment             | > 10 t/a   | If PBT/vPvB, further requirements are triggered under REACH, such as identification in SDSs or specific rules for CSA                           |

For substances registered between 10 and 100 t/a only a screening of PBT properties is possible, as both biodegradation and accumulation testing do not allow to compare results with the PBT/vPvB criteria of Annex XIII.

### 7.3.4 Conclusions on persistence and bioaccumulation

#### Chemical safety assessment

Persistence and bioaccumulation influence fate and behaviour of substances in the environment in interplay with the substance's mobility. They are core parameters for the assessment of organic substances, whereas for inorganic substances biodegradation is not relevant. Bioaccumulation is always expressed as BCF and hence available only from 100 t/a, if at all.

According to the ECHA criteria on the scope of exposure assessment, substances should be considered in CSA if they are either not readily degradable or have a  $\log K_{ow}$  above 3 /  $BCF > 100$ .

Abiotic degradation, expressed as half-lives in air and water are relevant for organic and inorganic substances and should be taken into account, if available.

In the tonnage band between 10 and 100 t/a substances with PBT/vPvB properties may not be recognized and hence the respective rules for safety assessment (minimization of emissions, no derivation of risk characterisation ratios - RCRs) not followed.

#### DPD<sup>+</sup>-method

The R-phrase R53 can be assigned alone or together with another environmental R-phrases. According to the rules of the DSD, the properties leading to R53 can be identified only if R53 is assigned alone. If an R53 is assigned to a substance in combination with other R-phrases, it is not clear from that classification if the substance is persistent or bioaccumulative or both.

Table 7.8: Criteria for R53/chronic toxicity in classification

| Classification                       | Criteria R53<br>Directive 67/548 |  |            | Criteria "chronic"<br>CLP Reg. |   |            |
|--------------------------------------|----------------------------------|--|------------|--------------------------------|---|------------|
|                                      | Rapidly degradable               | $\log K_{ow} \geq 3$<br>(except $BCF \leq 100$ ) | Connection | Rapidly degradable             | $\log K_{ow} \geq 4$<br>unless $BCF \leq 500$ | Connection |
| R 50/53; H410<br>Very toxic, chronic | X                                | X  | OR         | X                              | X   | OR         |
| R51/53; H411<br>Toxic chronic        | X                                | X  | OR         | X                              | X   | OR         |
| R52/53; H412<br>Harmful, chronic     | X                                |  | None       | X                              | X   | OR         |
| R 53; H413                           | X                                | X  | And        | X                              | X   | And        |

The log  $K_{ow}$  may influence the emission behaviour and the environmental fate of a substance. Therefore, knowledge of either parameter is important for identifying potential areas of risk. The actual persistence and bioaccumulation potential is not clear, if only the classification R53 is used. The use of test results, which are available either in the suppliers' information or the dissemination data base<sup>90</sup>, would give more transparency in the selection process.

The classification criteria for R53 correspond to the values proposed by ECHA for scoping the exposure assessment. If the classification of the CLP-Reg should be implemented in DPD+ (H-statements replace R-phrases), a gap would arise between coverage of classification and desired scope of exposure assessment in the area of bioaccumulation. Substances with a log  $K_{ow}$  between 3 and 4 (BCF between 100 and 500) would not be covered in the selection of lead substances.

The concentration limit for substances classified as R50 is defined differently by DPD+ (0.25% \* 3) than the classification rules for preparations (25%). The threshold for classification according to the DPD is 25% because a R50-substance can only trigger a classification of a preparation with R50<sup>91</sup>. According to DPD+, the absence of R53 (substance is readily degradable and does not bioaccumulate) for substances which are very toxic to aquatic organisms (R50) is considered by multiplying the limit concentration of R50/53 (0.25%) with the factor 3. This is justified by CEFIC as follows:

"R50 substances undergo rapid degradation and do not bioaccumulate. Hence, their risk [for] the environment is lower than that of substances labelled R50/53. According to Chapter R 16 of the ECHA Guidance on Information Requirements and Chemical Safety Assessment rapidly degrading substances [are destroyed in the] wastewater treatment plant [with an efficiency] of 67% whilst R50/53 labelled substances may not be affected (no degradation). This corresponding difference in the risk indicator can be accounted for by a correction factor of 3 in order to reflect the increased removal efficiency of a municipal wastewater treatment plant for rapidly degrading substances."<sup>92</sup>

This argumentation can in principle be supported but may be questioned with regard to mixtures which are used open in the environment (no STP connection).

*Identified weaknesses of DPD+: log  $K_{ow}$  and persistence are not considered in the selection of lead substances; only the aggregated information "R53" is used.*

*The use of the factor 3 for substances classified R50 is regarded as adequate although it may be questioned if emissions do not end up in an STP. The potential difference is believed insignificant<sup>93</sup> and the issue is therefore not further assessed.*

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<sup>90</sup>REACH Art. 112

<sup>91</sup> A classification „R51“ does not exist, a classification with „R52“ follows different rules. Therefore, only R50 is possible. CEFIC has used the classification threshold of R50/53 instead.

<sup>92</sup> CEFIC guidance, p. 12

<sup>93</sup> If the factor 3 was not applied, the concentration of substances classified R50 would be divided by 0.25 instead of 0.75. This is not likely to be the cause of overlooking significant risks in the selection of lead substances.

### 7.3.5 Information on ecotoxicity

Table 7.9 lists the information requirements on ecotoxicological substance properties and specifies for which registration tonnage it is required. End-point specific waiving options mentioned in the REACH Annexes are not discussed. The last column gives examples for the use of information in environmental risk assessment.

Table 7.9: Compilation of relevant information on environmental toxicity

| Hazard information  | Tonnage                 | Use of information / comments   |
|---|-------------------------|---|
| Acute toxicity to fish  | > 10 t/a                | $PNEC_{water}$  |
| Acute toxicity to crustaceans   | > 1 t/a                 | $PNEC_{water, marine}$ ; $PNEC_{sediment}$ and $PNEC_{soil}$ if no suitable other data available<br>For PBT-assessment: chronic test if $LC50 < 0,1$ mg/l<br>Algae: NOEC derived from the same test as LC50 |
| Acute & chronic toxicity to algae & other aquatic plants  | > 1 t/a                 |   |
| Inhibition of activity in sewage treatment plants   | > 10 t/a                | $PNEC_{STP}$  |
| Chronic toxicity to fish  | > 100 t/a               | $PNEC_{water}$<br>$PNEC_{water, marine}$ ; $PNEC_{sediment}$ and $PNEC_{soil}$ if no suitable other data available<br>Not for PBT/vPvB, if data on algae and crustaceans available                          |
| Chronic toxicity to fish:<br>a) early life stage<br>b) embryo and sac fry<br>c) juvenile growth | > 100 t/a               | $PNEC_{water}$<br>In-depth assessment of potential adverse effects  |
| Chronic toxicity crustaceans  | > 100 t/a               | $PNEC_{water}$ PBT/vPvB assessment  |
| Chronic toxicity sediment organisms   | > 1000 t/a              | $PNEC_{sediment}$   |
| Toxicity on soil micro- and macro-organisms   | > 100 t/a               | $PNEC_{soil}$   |
| Toxicity on invertebrates   | > 100 t/a<br>> 1000 t/a | $PNEC_{soil}$   |
| Toxicity on plants  | > 100 t/a<br>> 1000 t/a | $PNEC_{soil}$   |
| Long-term or reproductive toxicity to birds   | > 1000 t/a              | Secondary poisoning from aquatic and terrestrial food chain   |
| Toxicity on bees  | --                      | --  |
| Other known effects (Ozone depletion and formation, endocrine disruption etc.)                  |                         | Classification, assessment of non-toxic risks, assessment of "equivalent concern"   |

In the context of safety assessment under REACH the PNECs for most compartments are derived from the  $PNEC_{water}$ . Hence, in the lower tonnage bands, where specific test results on other organisms are missing, the toxicity for different protection targets is proportional to the aquatic toxicity.

The derivation of PNEC values is performed using the so called equilibrium partitioning method (EPM), where the ratio between the partitioning coefficient of the substance and the density of suspended matter is multiplied with the  $PNEC_{water}$ . Another method of deriving PNECs is the use of testing information and assessment factors; however this is possible only if that data is available.

The derivation of PNEC values cannot be applied for some groups of substances, because the correlation between properties and toxicity cannot be extrapolated by the equilibrium partitioning method. This concerns metals, substances with high ionization potential (e.g. salts), substances with  $\log K_{ow} > 5$  or surface active substances (tensides). For these substances, the aquatic

risk assessment does not “automatically” cover risks to sediments or soils; i.e. although no risk to the aquatic environment is identified, risks may occur to sediments or soils. In the ECHA guidance on information requirements respective RCRs for soils and sediments must be multiplied by the factor 10.

Table 7.10: List of environmental endpoints - PNECs, explanation and information needed to derive them

| PNEC                             | Protection target                            | Exposure compartment | Minimum data for direct derivation  | Derivation by modelling from                    | Comments  |
|----------------------------------|--|----------------------|---|---|---|
| Freshwater                       | Aquatic organisms                            | Surface water        | At least 1 short-term test from 3 trophic levels  | --  | Available at 10 ta  |
| Sediment                         | Benthic organisms                            | Sediments            | At least 1 long-term test with sediment organisms                                       | $PNEC_{water} \cdot K_{p_{soil-water}}$         | $EPM^{94} =$ screening                                    |
| Soil                             | Terrestrial organisms,                       | Agricultural soil    | At least 1 short term toxicity test on terrestrial organisms <sup>95</sup>              | $PNEC_{water} \cdot K_{p_{soil-water}}$         | Possible, pathway to groundwater                          |
| STP                              | Microorganisms                               | STP aeration tank    | Sludge respiration inhibition, nitrification inhibition etc.                            | --  | Many tests could be used                                  |
| Saltwater                        | Marine aquatic organisms                     | Sea water            | Tests with marine species   | $PNEC_{water}$<br>Factor 10                     | Available at 10 ta  |
| Marine sediment                  | Marine benthic organisms                     | Marine sediment      | At least 1 short term toxicity test on sediment organisms (fresh or saltwater)          | $PNEC_{water, marine} \cdot K_{p_{soil-water}}$ |   |
| Predators, oral (birds, mammals) | Fish eating predators, worm-eating predators | Fish, earthworm      | Acute or (preferred) long-term oral toxicity studies on birds or other mammals (NOAELs) | Ingestion studies, assessment factors           | Mostly no data, lipophilic substances and metal compounds |
| Groundwater                      | No method                                    | Groundwater          | No methods  | --  | No method   |
| Air (biotic)                     | Humans, terrestrial organisms                | Air                  | No methods  | Inhalation studies, assessment factors          | No method   |

For the following effects, no PNECs are available and no “traditional” risk assessment is performed.

Table 7.11: List of “other” environmental effects, explanation and information needed to derive them

| Type of endpoint     | Protection target         | Exposure compartment  | Minimum data for direct derivation             | Comments   |
|----------------------|---------------------------|-----------------------|--|--|
| Global warming       | Atmosphere                | “Earth”               | Gases contributing to GW known                 | Amounts from industrial chemicals may be relevant for a few gases, such as SF6 |
| Ozone depletion      | Atmosphere, all organisms | Atmosphere            | Halogenated organic compounds, Montreal list   | Covered by classification and RMMs as part of normal SDS development           |
| Ozone formation      | All organisms             | Air                   | Vapour pressure                                | VOC definition sufficient  |
| Long range transport | All organisms             | Air to water and soil | Persistence, half-life in air, vapour pressure | Half-life in air frequently not available                                      |
| Acidification        | Water, soil               | Air, water, soil      | PH-values; behaviour in the environment        | Amounts from industrial chemicals mostly not relevant.                         |

<sup>94</sup> Equilibrium partitioning method; the PNEC is regarded as valid for screening but may be misleading if Log Kow>5.

<sup>95</sup> E.g. plants, earthworms, microorganisms

### 7.3.6 Conclusions on ecotoxicity information

#### Chemical safety assessment

Information on the ecotoxicity of substances to organisms is essential for deriving PNEC values for the risk assessment. As a minimum acute tests from aquatic species from three different trophic levels are required to derive an aquatic PNEC.

PNECs for marine waters, sediments and soils can be derived from the aquatic PNEC if no testing information is available by using an assessment factor method. For the latter method, information is likely to be available only for substances registered above 100 t/a (testing proposals), if at all.

The PNEC to microorganisms is always to be determined independent of the aquatic PNEC. The PNECs derived using data and assessment factors are expected to be lower than the PNECs modelled using the equilibrium partitioning method.

According to the ECHA guidance, the risk assessment of the freshwater environment is regarded as covering the compartments soil and sediments, except the equilibrium partitioning method cannot be applied.

#### DPD+-method

If lead substances are selected based on the aquatic classification the hazardousness to marine organisms, soils and sediments is likely to be covered for most substances. However, risks from substances for which EPM cannot be applied (metals, surface active substances, and substances with  $\log K_{ow} > 5$  or a high ionization potential) may be underestimated. Risks from substances which are (more) hazardous to soil and sediment than to aquatic organisms may be underestimated as well. The toxicity to microorganisms, which may indicate problems in the sewage treatment plant, is not considered in the selection of lead substances.

Whereas classification defines "categories" of aquatic toxicity (below 1, between 1 and 10, between 10 and 100), LC50 values or PNECs give a more precise picture of the toxicity to aquatic organisms.

#### Example

Table 7.12: Example of differences in selection of substances using R-phrases or LC<sub>50</sub> values

| Substance | R-phrases | LC50 mg/l | C <sub>lim</sub> | C <sub>mix</sub> | LSI          | Result  |
|-----------|-----------|-----------|------------------|------------------|--------------|---|
| A         | R 50/53   | 0.5       | 0.25             | 15               | 15/0.25 = 54 | A = lead substance, although only <b>slightly</b> more toxic to aquatic organisms and contained in much <b>lower concentration</b> in the mixture |
| B         | R 51/53   | 1.5       | 2.5              | 50               | 50/2.5 = 20  |   |

In conclusion, information on the aquatic toxicity of substances can be regarded as a more precise measure than the classification. The information should be available for all substances via the internet; hence also if mixtures are used as input materials the formulator has access to these values.

Substances which are not classified but could be toxic to aquatic organisms may be overlooked, as has been described in detail in Section 0.

For substances to which the EPM does not apply risks to sediments and soils may be overestimated or underestimated<sup>96</sup>, as the partitioning and degradation behaviour would change due to differing bioavailability and degradation rates in the environment. This is an argument for including the log  $K_{ow}$  as separate indicator in the selection of lead substances, rather than having it (ambiguously) included by the R53.

The ECHA guidance on exposure assessment (part R 16) uses the human health classification based on testing of reprotoxicity and repeated dose toxicity as indicator of whether or not secondary poisoning may be relevant. This could be included in the selection criteria (as identification is done for the human health part of DPD<sup>+</sup> anyway) or as additional parameter to “check” the result of LSIs.

Risks to groundwater, the atmosphere and terrestrial organisms via air are not covered by R-phrases but may also not be detected in standard CSAs. The DPD<sup>+</sup>-method does not provide an option to consider respective information and hence, incentives to search for information are missing. Hence, criteria for these end-points could be included in the selection of lead substances.

*Identified weaknesses of DPD<sup>+</sup>: risks to sediments, soils or marine organisms may not be covered, in particular if PNEC derivation based on EPM-method cannot be applied, toxicity to STP (microorganisms) not considered; toxicity ranges of classification may lead to distortion*

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<sup>96</sup> The assessment of risks to the aquatic compartment covers those of sediments for substances with a log  $K_{ow}$  <5. If the log  $K_{ow}$  is > 5, the PEC/PNEC ratio is multiplied by 10 to take account of potential uptake of the substance by organisms via food. The assessment of risks for substances with high  $K_{oc}$  values takes account of several changes in bioavailability and degradation rates due to adsorption to organic matter. This applies analogously to soils.

## 8 RISK ASSESSMENT REPORTS

The review of risk assessment reports (RARs) carried out under the Existing Substances Regulation (ESR) further assesses if and which environmental risks are not indicated by the classification of a substance. It is another perspective on the question of which risks may be overlooked in the selection of lead substances by DPD<sup>+</sup> because it is founded on the aquatic classification.

All risk assessment reports (RARs) published on the website of the former European Chemicals Bureau (Ex-ECB<sup>97</sup>) were analysed in order to check, which types of risks could be overlooked by using the environmental classification as indicator for determining risks and for getting a general feeling of how the aquatic classification and environmental risks correlate. Two questions were assessed:

- Which types of risk are identified and which share of substances causing which risks are classified / not classified for the environment?
- What is the relation between risks for the compartments air, STP, soil and sediments and risks to the local aquatic environment?

Information compiled and evaluated was: Substance name and identity, classification (environmental R-phrases and CMR-classification), vapour pressure, log  $K_{ow}$ , water solubility and risk conclusions for the aquatic and terrestrial environment, the atmosphere, secondary poisoning and STPs.

Risk assessments under the Existing Substances Regulation (ESR) have been performed for prioritized substances and therefore do not reflect the average "normal substances". However, if substances have been prioritized because of their human health hazards, the environmental relevance can be regarded as "side effect" and "normal situation".

The RARs under ESR differ from the chemical safety assessment (CSA) under REACH in several aspects, such as the use of the total EU market volume as input amount<sup>98</sup>, the assessment of all known uses<sup>99</sup> and the consideration of cumulative effects in the environment<sup>100</sup>. Therefore, the results of EU risk assessments do not necessarily predict the outcome of a REACH-compliant CSA.

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<sup>97</sup> <http://ecb.jrc.ec.europa.eu/esis/index.php?PGM=ora>

<sup>98</sup> The risk assessment at EU level concerns the total amount placed on the market whereas under REACH only the registered amount must be considered by the registrant.

<sup>99</sup> In the EU risk assessment, all uses are to be assessed and the registrant only has to assess the identified uses that are known to him.

<sup>100</sup> The registrant does not have to consider emissions or exposures from substances placed on the market by his competitors. This means that any environmental risks that occur because of the accumulation of emission and exposures from all sources of use are not considered for registration; these have been subject to the EU risk assessment under the existing substances program.

## 8.1 Overview of the analysis

Of the originally planned 141 risk assessments under the existing substances program, 4 reports are not available to date<sup>101</sup> (total available = 137). For all other substances, the reports are available at least as draft version.

Due to resource constraints, only the RAR summaries could be screened and in a few cases, the main drafts were consulted. Only the risk conclusions ii) "There is at present no need for further information and/or testing and no need for risk reduction measures beyond those which are being applied already" and iii) "There is a need for limiting the risks; risk reduction measures which are already being applied shall be taken into account" were extracted from the reports. Further testing needs (conclusion i) were not followed up. If the risk conclusion iii) was drawn for at least one scenario in the EU risk assessment, this was counted as "risk" for the respective compartment.

Of the 137 analysed risk assessments, for 68 substances, at least one environmental risk has been identified<sup>102</sup>. For 4 metals several compounds were assessed (Zn: 6, Cd and Cr 3 and Ni 5 compounds). The risk conclusions for the compounds are equal, as they ionize in the environment and they are therefore counted as 1 substance. 2 metal compounds were assessed in addition (aluminium fluoride and diantimony trioxide).

Substances with an environmental classification (any single or combination of R50 to R53 or R59) were distinguished from substances without an environmental classification. Substances for which a classification is proposed in the risk assessment have been assumed as classified according to the proposal (one is proposed for classification with R54).

## 8.2 Conclusions from the RAR analysis

For 24 substances which are not classified for the environment, a risk has been identified in at least one scenario of the RAR. This confirms that substances can cause environmental risks even if they are not classified.

5 substances have been identified as PBT/vPvB. These substances are already included in the candidate list for authorization according to REACH. All of these are classified R50/53.

11 substances / substance groups are identified as SVHC on the candidate list for authorization<sup>103</sup> because of their CMR properties. One substance is on the candidate list because of being a PBT and a CMR (Pitch, coal tar). 9 of these SVHCs are classified also for the environment.

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<sup>101</sup> The assessment was performed in November 2010.

<sup>102</sup> An environmental risk means that in at least one of the scenarios calculated in the RAR the risk characterization ratio was > 1.

<sup>103</sup> This relates to the candidate list of November 2011.



Figure 3 shows the number of substances causing a particular environmental risk (atmosphere, STP, soil etc.). For each compartment the total number of risk conclusions is given (grey column) divided and it is distinguished if the substances are classified for the environment or not. It is evident from the figure that risks to the aquatic compartment are the most frequently identified, followed by risks to sediments, and soils. Risks to the atmosphere and risks for secondary poisoning occur the least frequent.

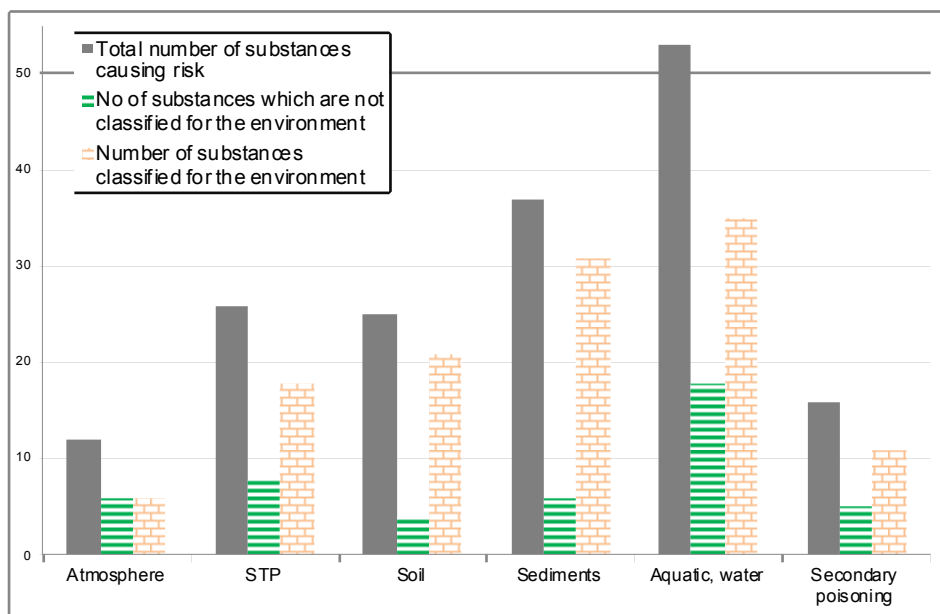


Figure 3: Number of substances causing risks (total # grey, # not classified green; # classified orange)

For the substances assessed in the EU risk assessments, the following can be learnt:

- approximately 50% of the substances causing risks to the atmosphere are not classified for the environment.
- approximately 30% of all substances causing a risk to STPs are not classified for the environment
- approximately 15% of all substances causing a risk to soil or sediments are not classified for the environment.
- approximately 35% of all substances causing a risk to the aquatic environment are not classified for the environment
- approximately 30% of all substances causing risks due to secondary poisoning are not classified for the environment.

68 substances were found to cause at least one environmental risk. Of these, 44 have an environmental classification (65%) and 24 are not classified for the environment (35%). Of the substances, which are classified, still in 25 cases at least one of the risks identified in the RAR was not obvious from the classification as illustrated by Figure 4.

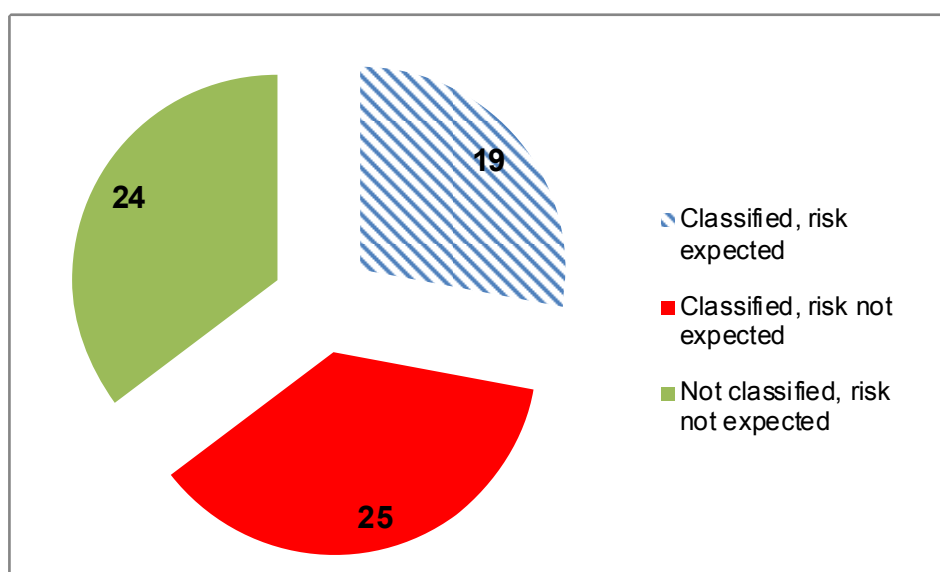


Figure 4: Predictability of risks from environmental classification

The decision of whether a risk is predictable or not based on the environmental classification was taken according to the following principles:

- If the substance is not classified (24)<sup>104</sup>, any risk identified in a risk assessment is regarded as “not predictable based on classification”
- If a substance is classified for aquatic toxicity without an R53 risks to the atmosphere (12) or to STPs (26) are regarded as not predictable based on classification. Risks to the aquatic environment are considered to be expectable.
- If a substance is classified with R53 alone or in combination with other R-phrases: risks to soils (0), sediments (2) and for secondary poisoning (0) are regarded as predictable based on classification.

<sup>104</sup> Figures in brackets indicate number of substances that have been identified. Some substances cause more than one of the mentioned risks unexpectedly, therefore the total of all numbers in brackets exceeds the total number of substances causing risks that could not be predicted from the classification.

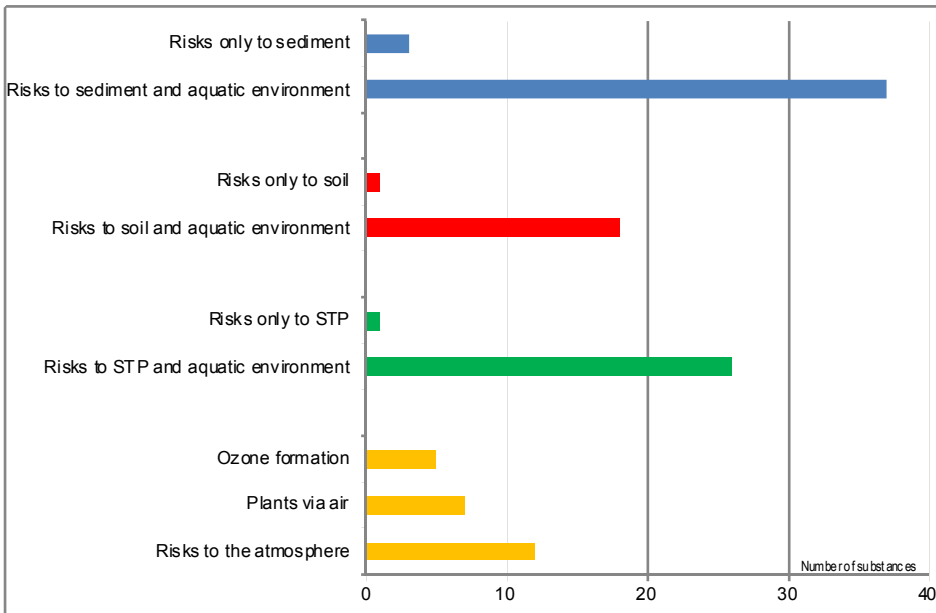


Figure 5 shows the correlation between risks to the aquatic environment and risks to other environmental compartments. For sediments (blue), soil (green) and STP (red) the number of substances causing risks to both compartments is illustrated next to the number causing risks only to sediment/soil/STP but not to the aquatic environment. In yellow the total number of substances causing risks to the atmosphere is differentiated into risks from ozone depletion and from exposure of plants via the air.

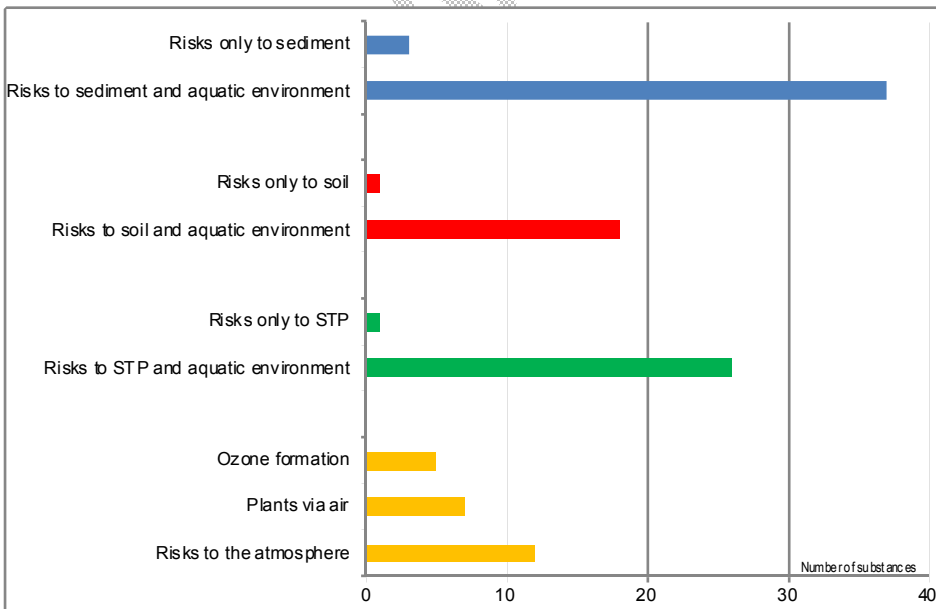


Figure 5: Overview of specific risks and coverage by aquatic classification

It can be concluded that most substances causing risks to sediment, soil or STP also cause risks to the aquatic environment. Hence, if the selection of substances would be based on the aquatic risks (not the aquatic classification!), risks to soils, sediments and STP should be expected and considered in the derivation of operational conditions (OCs) and risk management measures

(RMMs). However, for the majority of the substances were the EU risk assessment identified risks no environmental classification existed at all.

The following conclusions are drawn from the assessment:

- Risks to the atmosphere covered by RARs regard ozone formation and exposures of organisms via air. Risks related to long range transport and global warming are not explicitly mentioned.
- Substances causing risks to or via the atmosphere are not necessarily classified for the aquatic toxicity (6 classified and 6 not classified).
- Substances could cause risks to the STP even if they do not cause risks to the local aquatic environment (1) and if they are not classified as toxic to the aquatic environment (1).
- For the assessed substances, risks to soils and sediments appear to be correlated in terms of risk assessment with aquatic toxicity. There are very few cases where risks to soils (1) and sediments (3) have been identified but no risks for the aquatic environment.
- In most cases, the risks identified from the risk assessment would not have been expected from the environmental classification.

## 9 FINDINGS AND CONCLUSIONS ON DPD<sup>+</sup>

In this section the main conclusions on the applicability of DPD<sup>+</sup> for the consolidation of information on mixtures under REACH are compiled. The assessment and conclusions only relate to the environmental aspects of DPD<sup>+</sup>.

DPD<sup>+</sup> aims to support formulators in consolidating information from exposure scenarios (ESs) of substances used as input materials for a mixture. The workflow of DPD<sup>+</sup> can be divided into two distinct steps (c.f. Chapter 6):

- Step 1: selection of lead substances (LS) based on their classification, their concentration in the mixture and the classification limit values defined in the Dangerous Preparations Directive  
This step is described in detail in the CEFIC guidance document
- Step 2: use of the information on the conditions of use (CoU) in the ES of the lead substance to deriving the operational conditions (OCs) and risk management measures (RMMs) ensuring safe use for all the substances in the mixture.

The prioritization step (1) should facilitate the consolidation of information for the mixture, because less exposure scenarios need to be taken into account. This is justified, also according to the ECHA guidance, by the assumption that the overall risk of mixtures is determined by one (or a few) of its components and that therefore the adequate control of that substance ensures also that no risk occur from the other components of the mixtures.

The consolidating information on OCs and RMMs (2) is neither elaborated in detail in the CEFIC guidance on DPD<sup>+</sup> nor in the ECHA guidance for downstream users (DU). As concrete guidance and examples are missing, it was not possible to evaluate a methodological approach of DPD<sup>+</sup>. Nevertheless, some generic limitations of DPD<sup>+</sup> on identification of conditions of use were derived.

The findings and conclusions are separated according to the above mentioned two steps of DPD<sup>+</sup>. Each of the Sections includes proposals for how DPD<sup>+</sup> could be improved. Chapter 10 summarizes the results of a theoretical exemplification conducted using different consolidation approaches.

## **9.1 Limitations of DPD<sup>+</sup> in the identification of the risk determining substance**

The following sections summarize why the selection of an environmental lead substance according to DPD<sup>+</sup> may not result in the identification of the risk determining substance. If a substance is selected as lead substance, the conditions of use described in its exposure scenario are selected as conditions of use for the mixtures. Consequently, a wrong identification of a lead substance may result in operational conditions and risk management measures that don't adequately control the risks from the substances in the mixture.

### **9.1.1 Scope**

DPD<sup>+</sup> only considers substances which are classified. Non-classified substances may be disregarded in the assessment.

This interpretation is not fully in line with the interpretation of the legal text by the EU Commission, ECHA and the MS. Their understanding as laid out in the Guidance on the scope of exposure assessment implies that substances without a classification but indications that hazards could exist have to be considered in the exposure assessment and would therefore also be considered in the consolidation (Chapter 7.2).

The assessment of risk assessment reports (Chapter 8.2) showed that not all risks identified can be predicted based on the classification. This supports the view that also non-classified substances should be addressed.

Information on non-classified substances is not forwarded along the supply chain. Therefore, formulators only know which non-classified substances they use if they are used as such and not contained in a mixture. Even if a substance is used as such, no hazard information would be supplied. They may be able to request this information based on REACH Article 31(3).

Although non-classified substances may cause risks to the environment, the scope of DPD<sup>+</sup> is regarded as acceptable because it is pragmatic and manageable for the formulators. The issue may be reconsidered at a later stage.

### **9.1.2 Foundation on classification**

The limitations of DPD<sup>+</sup> due to its foundation on the classification can be divided into two parts: shortcomings because of the classification approach and shortcomings because of the considered hazards. Whereas the first part addresses the methodology as such, the second discusses details within that structure.

Limitations because of the system of classification

### Category approach

The classification of substances is based on ranges of aquatic toxicities and related assignment of R-phrases. Concentration ranges of classified substances are used to classify the mixtures. These two types of groups or categories lead to sudden, step-wise changes in the classification of substances and mixtures<sup>105</sup> (Chapter 7.1.).

This category approach of classification influences the size of the LSI both via the classification as such and the value of the limit concentration. This may mislead the ranking of risk determining substances: the toxicity of two substances classified with different R-phrases may be very similar and the resulting LSI values would differ by the factor 10 only because of the use of different limit concentrations as divisors in the different classification category (c.f. Table 7.12)

DPD<sup>+</sup> could be improved by changing the values used to derive the lead substance indicator. The lead substance indicator concerning the aquatic environment should be expressed as concentration in the mixture divided by the lowest result from toxicity testing of the substance:

$$LSI = Conc_{mx} / LC_{50}$$

In order to cover the gap between classification and potentially risk causing substances, substances with LC<sub>50</sub> values exceeding 1 mg/l which are readily degradable should be considered<sup>106</sup>.

### Mobility of substances

The classification of substances is hazard based and the mobility of substances, which determines how they are emitted and where they end up in the environment are not covered. This is well justified for the classification rules, because they are intentionally not considering risks.

In the case of DPD<sup>+</sup> the risk determining substance is to be identified and therefore mobility properties, such as water solubility, vapour pressure and LogKow<sup>107</sup>, are relevant in order to develop meaningful lead substance indicators. The ECHA guidance for downstream users also recommends the use of mobility information for the identification of critical components.

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<sup>105</sup> LC50 of 0.9 mg/l leads to classification with R50 and a limit concentration of 0.25; LC50 of 1.1 mg/l leads to classification with R51 and a limit concentration of 2.5.

<sup>106</sup> Currently substances classified R52 are not included in the method and substances with R51 do not exist according to the classification rules of DSD and DPD.

<sup>107</sup> The logKow is part of the information needed to assign the R-phrase 53. However the R53 is ambiguous and therefore, this property is included here.

If physico-chemical properties are not considered, substances may be identified as lead substance only based on their (high) concentration in the mixtures but may be emitted in negligible amounts on the emission pathways relevant for the use (c.f. Chapter 7.3.1).

The selection of lead substances by DPD<sup>+</sup> could be improved if these mobility properties were included. In order to relate the concentration in the mixture to the emission potential and a particular emission pathway (and hence the options of emission controls) the PC parameters water solubility (emission to water), logKow (partitioning and adsorption to (sewage) sludge) and vapour pressure (emission to air) should be included in the selection procedure. They may be modifiers of the initial selection of LSIs.

### **Persistence and bioaccumulation**

A substance's logKow and degradability are implicitly included in the classification via the assignment of R53. It is not always clear which of the two properties trigger the classification (c.f. Chapter 7.3.3).

Both parameters influence different aspects of potential environmental risks. In particular the risks to sediments and soils may be higher for persistent and bioaccumulative substances. This is e.g. taken into account in the chemical safety assessment for the derivation of risk characterization ratios for sediments and soils. The ECHA guidance for DU recommends considering the persistence and bioaccumulation potential in the identification of critical components.

DPD<sup>+</sup> could therefore be further improved, if the both properties are considered in the selection of the lead substance. This could be implemented as follows:

- LogKow and degradability are explicitly included as selection criteria for lead substances
- if log Kow > 5, the LSI should be multiplied by the factor 10.
- the LSI should be divided by 3 for all substances, which are readily degradable, as currently implemented in DPD<sup>+</sup> for substances classified with R50.

#### **Limitations related to the consideration of hazards**

The classification system does not address all environmental risks because related hazard endpoints are partly missing (c.f. Chapter 7.3.5).

Classification categories for environmental hazards to or via the atmosphere, except for ozone depletion (R59) don't exist, because no respective endpoints are defined or have been operationalized. No hazards for terrestrial organisms are considered.

Some hazards, such as the toxicity to sediments and soils are generally regarded as covered by the classification of aquatic toxicity but may be underestimated, e.g. where the equilibrium partitioning method cannot be applied. Risks to microorganisms in the STP may be overlooked, as respective



toxicity not necessarily corresponds to the aquatic toxicity of a substance<sup>108</sup> (c.f. Chapter 8).

DPD<sup>+</sup> has the same shortcomings with regard to the coverage of environmental risks, because of its foundation on the classification system. In addition the classification as ozone depleting substance is also not included in the criteria for a lead substance.

Respective improvements of DPD<sup>+</sup> could be the following modifications to the method for identifying lead substances<sup>109</sup>:

- The pathway and protection target air / atmosphere should be added as second, separate lead substance selection category; i.e. two lead substances per mixture should be selected, one for water and one for air.  
Criteria for deriving an LSI for the atmosphere would have to be developed, as no analogy with the aquatic toxicity can be established, because no limit concentrations for classification of mixtures exist<sup>110</sup>.
- The toxicity to microorganisms should be checked and compared to the aquatic toxicity of the lead substances to ensure that risks to STPs are not overlooked. This could be an additional selection criterion.
- It could be considered to include substances classified as reprotoxic or which show repeated dose toxicity and are not readily degradable and have a log Kow > 3 to ensure that effects on the food chain are considered. An integration of substances classified as CMRs may be considered.

## 9.2 Limitations of DPD+ in consolidating OCs and RMMs

According to DPD<sup>+</sup> the operational conditions (OCs) and risk management measures (RMMs) of the lead substance's (LS) exposure scenario (ES) are copied to the ES for the mixture<sup>111</sup>. In a second step the consistency of information should be ensured (c.f. Section **Fehler! Verweisquelle konnte nicht gefunden werden.**). Since normally only one environmental LS is selected the consistency check is not likely to change the RMMs but may lead to changes in OCs, because of the consolidation for occupational health<sup>112</sup>. Consequently, the OCs may differ but the RMMs in the ES of a mixture are in most cases the same as described in the ES of the LS. Due to this, formulators

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<sup>108</sup> The analysis of risk assessment reports showed that out of 26 substances posing risks to the STP only 1 didn't cause risks in the aquatic environment. This indicates that normally the toxicity to microorganism correlates to a toxicity to the aquatic environment. However, the assessment cannot be regarded as representative and more substances should be compared.

<sup>109</sup> For improvement proposals related to the coverage of soil and sediment toxicity by the aquatic classification see the Chapter on persistence and bioaccumulation.

<sup>110</sup> The LSI is derived by dividing the actual concentration of a substance in the mixture by the concentration limit for classification. If more than one substance potentially causing risks to the atmosphere are contained in the mixture, an LSI would be necessary to prioritize which of these is to be considered for the consolidation of RMMs.

<sup>111</sup> REACH does not require the preparation of an ES for the mixture. Apart from providing a consolidated mixture ES it is also possible to forward the individual substance ESs received or include information in the main body of the SDS.

<sup>112</sup> 3 lead substances are identified for human health and hence, 3 sets of operational conditions are compiled together with those, which are selected for the environmental LS.

consolidating according to DPD<sup>+</sup> may be formally non-compliant and risks to the environment may not be adequately controlled.

Apart from this, there are some other reasons why adequate control of risks may not be achieved by consolidation based on DPD<sup>+</sup>, which concern the dependency of emission pathways and RMMs on substance properties (c.f. Chapter 9, final report). It is important to note that the formulator is not legally required to check if the CoUs he receives for the substances ensure that risks are adequately controlled. However, in order to ensure that he forwards useful information "in an adequate form" to his clients he may consider taking more responsibility than required.

### 9.2.1 Formal non-compliance and factual risks

The conditions of use are defined for each substance separately and they are separately binding for any downstream user<sup>113</sup>. Adequate control of risks is achieved if the risk characterization ratio (RCR), which is the quotient of a substance's predicted environmental concentration (PEC) and predicted no effect concentration (PNEC) remains under the value of 1. Only if the conditions of use for the mixture cover all conditions of use (CoU) received with the input materials, the formulator can rely on that the RCR remains under 1 for all substances in the mixture.

DPD<sup>+</sup> disregards the conditions of use which are defined and recommended for any substance other than the lead substance. Although these substances may not determine the overall risk, it is still formally required to ensure that also their conditions of use are implemented and communicated.

Consequently, without checking that all conditions of use received are covered by the conditions of the lead substance, the formulator risks being formally non-compliant with REACH using DPD<sup>+</sup>. A refined scope and aim of the consistency check including a cross check with all received information and potential revisions of conditions, if necessary, could solve this problem.

### 9.2.2 Appropriateness of RMMs

RMMs are appropriate when they achieve the intended emission or exposure reduction (efficiency) and when it is feasible to implement them in a given process. The following core aspects are relevant for determining a RMM's appropriateness<sup>114</sup>:

- 1) The efficiency of most environmental RMMs depends on the properties of the substances to be treated. For example, there is no biodegradation of metals or inorganic compounds and volatile substances are not easy to contain in landfills etc. Hence, for different substances in a mixture the same RMM has a different efficiency.

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<sup>113</sup> The term safe use of "a substance as such, in mixtures or in articles" is used. The duties to identify, implement and recommend the safe CoU apply to the individual substances.

<sup>114</sup> Approaches for the selection of appropriate RMMs are explored in an ongoing project by the German UBA "Efficiency of risk management measures for emission reduction" (FKZ 3711 63 419)

- 2) The type of the process and the mobility properties of substances determine how a substance is emitted from the process.
  - a. The efficiency of RMMs needs to take into account which fraction of the emitted substance is actually captured and treated by the device. This is frequently not considered.
  - b. Risks may occur in different compartments than the emission pathway. Therefore, for example substances that deposit from air may cause risks in surface waters but RMMs are needed for the air pathway.
- 3) RMMs may be incompatible with certain emission types (e.g. ultrafiltration should not be used for water emissions with a high share of solid particles) and is hence inappropriate for certain processes
- 4) The efficiency of RMMs may be reduced by certain substances, e.g. some substances may be catalyst poisons or increase another substances solubility thereby preventing sedimentation in water treatment.
- 5) In practice, some RMMs are state of the art, others are only applied in specific cases; combinations of measures may preferred over highly efficient single RMMs and vice versa.

Formulators using DPD<sup>+</sup> who only check the consistency between selected lead substances may risk not being in conformity with the requirements to forward information along the supply chain.

If DPD<sup>+</sup> were implemented with a completeness check that considers all substances' information, the formulator would select the strictest OCs from all received ESs and may either

- select the RMM with the highest efficiency or
- formally "add up" all different RMMs.

If the RMM with the highest efficiency was selected, all aspects listed above may apply and, apart from a potential legal incompliance, lead to both lack of factual control of risk for some of the substances and the selection of a RMM which is not appropriate for the process. The latter is however only likely to occur in cases, where the operational conditions are defined so widely that fairly different processes could be covered<sup>115</sup>.

If all RMMs were added up, legal compliance would be definitely achieved but appropriateness is not ensured as the approach is overly conservative and not likely to be implemented by any DU.

### 9.2.3 Conclusions on the selection of CoUs

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<sup>115</sup> E.g. the PROC 7 – industrial spraying may be used to define the process; different types of the process could be understood, such as electrostatic powder coating or lacquering with high pressure guns. The former would require quite different RMMs than the second.

The current description of DPD<sup>+</sup> does not ensure legal compliance in all cases, because it is not explicitly prescribed to check that the conditions of use of any substance for which respective information is received is covered by the information forwarded with the mixture.

The problem of legal compliance could be solved by including all substances in the consistency check. This is e.g. described in the "REACH Practical Guide"<sup>116</sup> of the German VCI (c.f. Section 6.4), which proposes that checks should be performed to ensure that all risks from the mixture are adequately controlled. These checks would involve the assessment of whether or not all ESs are considered appropriately in the information for the mixture and also to include substances, for which no ES exist but which are relevant with regard to environmental risks.

If such a consistency check would simply lead to the result that all RMMs are listed for the mixture this "solution" would result in set of RMMs which often may not be implementable in practice. Consequences would be communication up the supply chains in order to have the chemical safety assessment refined, formulators conducting DU CSRs, the cease of uses or non-compliance of DUs.

So the analysis not only shows that a prioritization approach like DPD<sup>+</sup> is partly insufficient to ensure compliance and control of risk but also highlights the challenges in defining appropriate risk management measures and poses the question of which actor in the supply chain is able (and can take the responsibility) for the identification of such adequate RMMs (c.f. recommendations in Section 11).

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<sup>116</sup> CEFIC/VCI: REACH Practical Guide on Exposure Assessment and Communication in the Supply Chains Part III: Mixtures under REACH, March 2010. Available at: [https://www.vci.de/Downloads/REACH\\_Practical\\_Guide\\_Part\\_III\\_07\\_2010\\_en.pdf](https://www.vci.de/Downloads/REACH_Practical_Guide_Part_III_07_2010_en.pdf)

# 10 EXEMPLIFICATION OF CONSOLIDATION APPROACHES

## 10.1 Work process of exemplification

The aim of the exemplification performed during the project was to analyse the work processes and results for consolidating information on safe conditions of use (CoU) including risk management measures (RMMs) using the different approaches: DPD<sup>+</sup>, an improved DPD<sup>+</sup> (DPD<sup>+</sup>-rev) and a non-prioritizing approach.

DPD<sup>+</sup> was applied as interpreted from the CEFIC guidance document (c.f. Chapter 6); hence specific approaches of companies which applied DPD<sup>+</sup> are not taken into account.

The recommendations derived from the analysis of DPD<sup>+</sup> for an improved selection of lead substances were operationalized by developing additional or revised selection rules and selection criteria called DPD<sup>+</sup>-rev.

An approach not involving a prioritization of substances was outlined as third alternative approach. It was based on the use of in-house knowledge and the consideration of all information on all substances at the beginning of the consolidation process.

The analysis of the approaches consisted of:

- the development of two generic use descriptions (metal cutting and textile finishing)
- the description of six substances with different PC and (eco-)toxic properties,
- the development of an ES for each of the six substances in both uses (12 substance ESs, 6 for metal cutting and 6 for textile finishing)
- the definition of two mixtures containing six fictive substances each
- the consolidation of the substance ESs for the two mixture using the three different approaches
- the comparison of differences in procedures and results due to using the three approaches for consolidation.

Due to the "laboratory" character of the exemplification the definitions of substance properties, the combinations of substances in the mixtures and the CoU are partly theoretical, but closely related to reality.

The format of the ESs was only used to finally compile the information on safe conditions of use of the mixture to be forwarded in the supply chain because it is a well-established and well-structured format. Under REACH the formulator has different options of how to provide information to his customers and is not required to provide an ES with the mixture.

It should be noted that the examples were designed to highlight specific issues expected to be challenging in the consolidation of information. To which extend the identified issues and difficulties will occur in “real-life”-situations can therefore not be predicted and may need to be analysed in other projects.

The details of the exemplification are described in detail in a separate background report. The following sub-chapters include the main facts used for this detailed analyse and the conclusions drawn from it.

## 10.2 Workflow of non-prioritizing approach

The exemplification followed the workflow in Figure 2 for DPD<sup>+</sup> and DPD<sup>+</sup>-rev. The workflow for the alternative approach illustrated in the following.

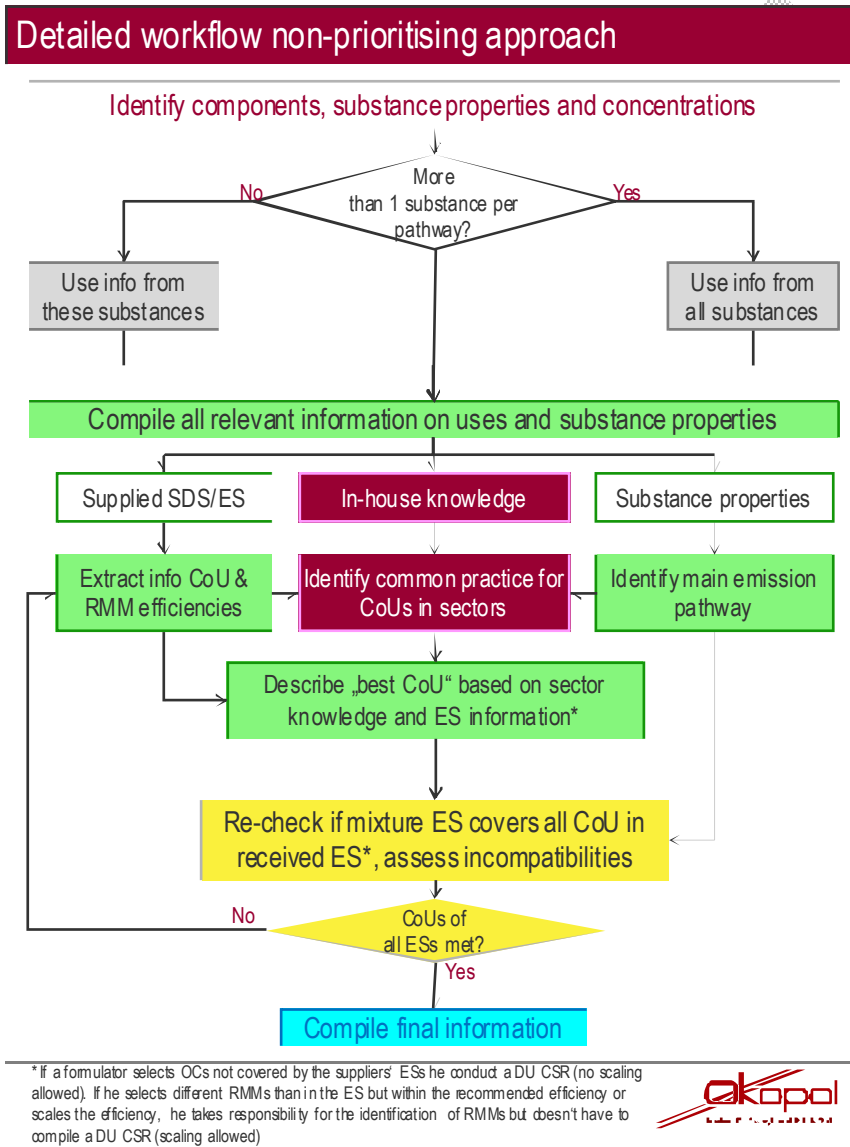


Figure 6: Workflow of the non-prioritizing approach tested in the exemplification

### 10.3 Illustration of examples

The core factual results of the exemplification confirm the conclusions on the limitations of DPD<sup>+</sup> from the generic assessment (c.f. Section 9.2) regarding the selection of CoUs. The following two tables illustrate these findings for the textile finishing agent. The first table illustrates DPD<sup>+</sup>, the second the non – prioritizing approach. The tables should be read from the left to the right.

In the first two columns of both tables, the RMMs for water emissions and air emissions are quoted from the suppliers' ES. In the orange shaded columns, for DPD<sup>+</sup> the initial RMMs selection from the lead substances ES is presented and for the non-prioritizing approach the RMMs according to sector and process knowledge are given. In the grey shaded columns, the RMMs are presented which would be selected after a consistency check aimed at legal compliance. For DPD<sup>+</sup> in addition the selection is presented that would result if only the RMM with the highest efficiency was chosen.

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Exemplification

Table 10.1: Illustration of RMM selection according to DPD+ in a modeled textile finishing mixture

| Substance  | RMM in ES of supplier for air        | RMM in ES of supplier for water   | RMM in mixture ES from lead substance (air) | RMM in mixture ES from lead substance (water)                  | Consistency check (formal compliance) (air) | Consistency check (formal compliance) (water)                  | Consistency check selecting only strictest measure by efficiency | Consistency check selecting only strictest measure by efficiency            |
|--|--------------------------------------|---|---|--|---|--|--|---|
| A (organic)  | Thermal oxidiser efficiency > 90%    | Biological treatment acc. to degradability (87% )                                 | Not needed                                  | Precipitation efficiency > 95% and filtration efficiency > 95% | Thermal oxidiser efficiency > 90%           | Biological treatment acc. to degradability and                 | Substance B is not considered because it is not classified       | Substance B is not considered because it is not classified                  |
| B (volatile organic); hazardous but not classified | Thermal oxidiser efficiency > 99.99% | Biological treatment acc. to degradability (67% ) and filtration efficiency > 99% |   |  | B not considered as not classified          | Filtration efficiency > 99% and                                |  |   |
| C (organic)  | Not needed                           | Ultrafiltration efficiency > 80%  |   |  | Carbon filter efficiency > 95%              | Precipitation efficiency > 95% and filtration efficiency > 95% |  |   |
| D (volatile organic)                               | Carbon filter efficiency > 95%       | Filtration efficiency > 85%   |   |  | Not needed                                  | Ozone oxidation efficiency > 90%                               |  |   |
| E (metal)  | Not needed                           | Precipitation efficiency > 95% and filtration efficiency > 95%                    |   |  |   |  |  |   |
| F (organic)  | Not needed                           | Filtration efficiency > 92% and ozone oxidation efficiency > 90%                  |   |  |   |  |  |   |
| <b>Lead substance acc. to DPD+</b>                 |                                      |   |   |  |   |  | Precipitation efficiency > 95% and filtration efficiency > 95%   | <i>RMM may not be sufficient for the removal of the organic substance F</i> |

Table 10.2: Illustration of RMM selection according to a non-prioritizing and sector knowledge based approach in a modeled textile finishing mixture

| Substance                             | RMM in ES of supplier for air        | RMM in ES of supplier for water   | Selection by sector knowledge air   | Selection by sector knowledge water   | Check of ES coverage (air)                                | Check of ES coverage (water)   |
|---------------------------------------|--------------------------------------|---|---|---|---|--|
| A (organic)                           | Thermal oxidiser efficiency > 90%    | Biological treatment 87% acc. to degradability                                    | Thermal oxidiser eff. 99.8% with exhaust filter for particles / metals eff. 80 – 95% depending on substance | Precipitation eff. metals & organics 95% ; filtration and biological treatment (eff. acc. to degradability) | OK  | OK   |
| B (VOC); hazardous but not classified | Thermal oxidiser efficiency > 99.99% | Biological treatment acc. to degradability (67% ) and filtration efficiency > 99% |   |   | OK  | OK; filtration efficiency ensured due to additional precipitation step (responsibility of selection of RMM shifts to formulator) |
| C (organic)                           | Not needed                           | Ultrafiltration efficiency > 80%  |   |   | OK  | OK   |
| D (VOC)                               | Carbon filter efficiency > 95%       | Filtration efficiency > 85%   |   |   | May be critical, detailed substance specific check needed | OK   |
| E (metal)                             | Not needed                           | Precipitation efficiency > 95% and filtration efficiency > 95%                    |   |   | OK  | OK; filtration efficiency may have to be verified  |
| F (organic)                           | Not needed                           | Filtration efficiency > 92% and ozone oxidation efficiency > 90%                  |   |   | OK  | OK; oxidation covered by biology and precipitation   |



The exemplification shows differences in the selection of RMMs and illustrates the compliance and practical issues discussed before. It is notable that the substance B, which requires strict RMMs for air would, due to a missing aquatic classification, not be considered by DPD<sup>+</sup>. It can be seen that the lead substance not necessarily has the ES with the strictest RMMs and the differences in applicability of RMMs are particularly apparent when comparing the measures for metals and for organic substances.

Furthermore, the examples once more illustrate that the communication of specific RMMs rather than only required efficiencies by the registrant may even cause more problems than it supports the formulators. Related to that it is apparent, that the core question of obtaining the efficiency of RMMs in relation to specific substances (substance properties) is an issue which cannot be resolved by consolidation but needs separate attention.

#### **10.4 Main findings from the exemplification**

The consolidation of information according to DPD<sup>+</sup> and DPD<sup>+</sup>-rev included an initial information compilation and a “final consistency check”, which was performed assuming that the formulator aims to achieve conformity with REACH spending the lowest resources possible.

The overall resources needed for the consolidation process according to DPD<sup>+</sup> and DPD<sup>+</sup>-rev mainly depend on the quality of the consistency check. If that check is conducted in detail the efforts are similar to those needed for the non-prioritizing approach. In this case only the stage of the consolidation differs (DPD<sup>+</sup>/DPD<sup>+</sup>-rev at the end, non-prioritizing approach at the end).

The usefulness of prioritization with regard to saving time and expertise can therefore be questioned if high quality information should be developed for the mixtures.

The initial selection of OCs and RMMs according to DPD<sup>+</sup>/DPD<sup>+</sup>-rev does not always ensure adequate control of risk and coverage of all ES. This was illustrated in the example by obviously assigning RMMs to substances for which they are not applicable or by failing to consider RMMs for the air pathway. It clearly showed that a formulator who does not carry out a thorough consistency check, may not be in compliance, because the ES for the mixture does not cover all conditions of use of the exposures scenarios of the contained substances.

As a second step, the consistency checks for DPD<sup>+</sup> and DPD<sup>+</sup>-rev were carried out with “minimum effort”. This means that the RMMs’ efficiencies for all substances were compared to the efficiency of RMM of the lead substance. When the lead substance’ RMMs had lower efficiencies than those of other substances, the RMMs of the other substance and their efficiencies were simply added to the ES. This led to formal conformity with the REACH requirements: the conditions of the received ESs were all covered. However, the final selection of measures is regarded as not appropriate because

- The measures may not be compatible with either the type of emissions (e.g. activated carbon filter recommended for aerosol emissions) or the

types of substances in the emission (e.g. oxidation of wastewater containing organo-halogens with ozone)

- the measures are overly strict (e.g. several measures combined) and the needed efforts are not necessary to ensure control of risks

Consequently a “half-hearted” consistency check may ensure legal compliance but may fail to ensure appropriateness of measures. Only a thorough check considering also the applicability of RMMs to the different substances, the emission pathways of substances from the mixture and the current practice in the end-using sector may derive useful information on the conditions of use for a mixture.

The conclusion from the above outlined findings is that the quality of the consolidated information on OCs and RMMs for the mixture mainly depends on the quality and depth of the consistency check. If the consistency check:

- is not done at all the selected CoUs are very likely to either not cover all risks from substances in the mixture (incompliance) or to be not implementable in practice (inappropriate).
- is done at a “medium quality level” (RMMs are added up to ensure coverage of all ESs), the CoUs are likely to be overly strict.
- is done at a high quality level also the CoUs are expected to be of high value and ensuring safe use. This consistency check resembles the first steps of the non-prioritizing approach.

Whether the evaluation of all information is performed at the beginning (non-prioritizing approach) or the end (“DPD+ with high quality consistency check”) of the process doesn’t make a big difference with regard to compliance.

Both approaches are manageable if the CoUs received in the suppliers’ ESs are comparable in structure and content. Whereas the RMMs only concern the emission from the process, the OCs determine how a substance is to be applied. The OCs should not be subject to scaling<sup>117</sup>. If the CoUs of the input materials’ ESs differ the formulator needs to take action to bring the ES into a comparable format<sup>118</sup>.

The non-prioritizing approach is likely to derive more realistic CoUs if combined with in-house knowledge from the formulator at an early stage of the process. This could be further supported if the registrant communicated needed RMM efficiencies rather than detailed technical types of measures because the process of selecting appropriate RMMs by the formulator may be simpler if he first identifies the most frequently applied measures and then checks, if the required (substance-specific) efficiencies of emission reduction can be achieved for any of the relevant components.

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<sup>117</sup> Scaling is the modification of conditions of use in an exposure scenario by a downstream user in cases, where the actual use differs from the conditions in the ES but is believed to remain within the scope. Regarding the environment scaling is understood as applicable to the efficiency of RMMs and the environmental conditions, e.g. lower or larger dilution volumes in rivers etc. For more information see for example <http://www.umweltdaten.de/publikationen/fpdf-14224.pdf>

<sup>118</sup> This situation is similar to a “use not covered by the ES”; the formulator may scale the conditions which can be scaled or conduct a DU CSR or communicate with his supplier or stop the use of the substance.

The (legal) consequences regarding a possible shift of responsibility for the identification of RMMs from the registrant to the DU if the registrant only recommends required efficiencies and the formulator identifies the specific technical measure were not subject to the study, but should be further explored to inform the discussion on this possible future option.

The need to consider all information is obvious for the non-prioritizing approach. It is not so obvious but rather "hidden in the consistency check" for DPD+. In particular an IT-implementation of DPD+ may bear the risk that the results are not quality checked in such a way by the users.

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## 11 RECOMMENDATIONS

Based on the conclusions from the project the consultants developed the following set of recommendations.

### **Open discussion with the chemical industry**

The results of the analysis of DPD<sup>+</sup> should be discussed openly with the responsible persons/working groups at CEFIC. The aim of a discussion should be to raise awareness and a common understanding of the identified shortcomings of the method.

It should be communicated that an improvement of the identified weaknesses of DPD<sup>+</sup> may not resolve the core challenge of the identification and selection of appropriate environmental RMMs. The substance-specific efficiencies of RMMs and the influence of the mobility of substances on their emission pathways from processes and in the environment require that the identification of conditions of safe use consider all information on substances potentially causing an environmental risk. This contradicts an approach to prioritise information for further use.

It should be pointed out that the use of DPD<sup>+</sup> may result in the communication of CoUs which are not covered by the received ESs, and that formulators would run the risk of non-conformity with REACH.

### **Avoid integration of DPD<sup>+</sup> in IT-tools if thorough quality checks cannot be ensured**

The problem of non-conformity with REACH may be particularly relevant, if DPD<sup>+</sup> or other prioritising approaches are integrated in IT-tools, because the users normally do not actually reconstruct the logics of automated consolidation, and are not likely to carefully review the outcome of such computer-generated information.

With view to the fact that an effective consistency check is necessary for the initial consolidation results of DPD<sup>+</sup> and that the consolidation of conditions of use is in general difficult to standardize, an IT-implementation at the current time may not be helpful at all.

### **Involve the downstream user industry**

The result of the generic analysis and the modelled exemplification of DPD<sup>+</sup> should be communicated to the downstream user industries, in particular to the formulators of mixtures. They should be made aware of the limitations of DPD<sup>+</sup> and the need to conduct a thorough consistency

check if the method is applied, in order to ensure formal conformity with the ESs.

Secondly and even more important is the discussion on the standardized descriptions of use by formulators and end-users of mixtures up the supply chain, in order to harmonize ESs received from suppliers. This approach of “making a use known to the supplier” has proven to be effective<sup>119</sup>. This could generate the following benefits:

- Registrants would be supported in their registration process. This may be particularly important for the second registration deadline, as more small and medium sized enterprises are expected to register.
- OCs would be communicated in a harmonized way, facilitating the checking of coverage of ESs by formulators’ and end-users.
- Described OCs and release factors may be less conservative than ERCs or spERCs reducing the need for additional RMMs
- Formulators would receive appropriate RMM recommendations instead of theoretical technically described measures which cause difficulties in consolidation.
- Appropriate and already implemented RMMs would be recommended rather than measures which are not practical or overly strict.

Downstream users may once more consider how a sector-wide process of compiling information on uses could be organized and in which form information could be provided upstream to registrants. One difficulty currently faced in this discussion is that there is little confidence among DUs in the readiness and the available resources of suppliers to work with information provided from downstream. Hence, one precondition for the DUs’ motivation would be a clear commitment of registrants to work with the DUs, e.g. in specific information exchange fora.

### **Discuss responsibility for the identification of RMMs**

The project showed that consolidation of information is more difficult if specific RMMs are recommended by the registrant and may even result in wrong, inapplicable or incompatible measures. Therefore a discussion is needed about which actors should actually identify the appropriate technical measures.

Under REACH formulators are neither to make exposure assessments nor to calculate risk characterization ratios or to identify the conditions that ensure adequate control of risk for single substances. This is clearly the task of the registrant. However, this project showed that an approach where the formulator defines the technical specification of RMMs that

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<sup>119</sup> In the exemplification, the conditions of use were described in a similar way for each of the two examples which can be regarded as all suppliers having used the same format for providing their exposure scenarios. The information was compiled at a higher level of detail than e.g. the spERCs and could represent an example of how DUs would make their use known to a supplier. This facilitated the consolidation of information significantly.

achieve an efficiency of emission / exposure reduction which is calculated and communicated by the registrant may be useful to develop practical and meaningful information on risk management. This would also better ensure that the measures suits to the process, all substances in the mixture and the mixture as a whole and achieves the necessary emission and exposure reduction<sup>120</sup>.

Another approach would be to have an informal and iterative information exchange between registrants and formulators based on exposure scenarios before registration or formal communication via the SDSs.<sup>121</sup>

### **Further activities**

The further development or support of DPD<sup>+</sup> is not recommended based on the results of this project. However, the generation of knowledge and experience in the consolidation process using real-life substances and mixtures is of high priority to identify where (standardized) support tools could be developed and how they could look like. An analysis of challenges faced by the formulators applying non-prioritizing approaches and “manually” consolidating ESs of registered substances is yet missing. Respective activities in example sectors should be launched soon, in order to be able to provide results before the second registration deadline.

The most important step to follow-up on this work, which does not necessarily requires real-life eSDSs would be to develop guidance and tools for formulators to assess the appropriateness and efficiency of risk management measures. This could be in the form of an excel table listing different types of (end-of-pipe) risk management measures with a specification of which efficiency could be reached for which (group) of substance<sup>122</sup>.

### **Mixture toxicity**

In the context of the project also a small research on methods to assess the mixture toxicity was conducted and the results evaluated with regard to their usefulness in the consolidation of information on mixtures.

DPD<sup>+</sup> is not intended for the assessment of mixture toxicity and it therefore also not suitable. Furthermore, the joint action of substances is not covered by any of the current provisions under REACH except for some very vague formulations in the context of the chemical safety assessment.

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<sup>120</sup> Such an approach may be interpreted as a partial shift of responsibility from the registrant to the downstream user with respective legal consequences. Further elaboration on such legal issues was not part of the project

<sup>121</sup> . However, this may be more complex for the formulator (many input materials) and difficult, as some substances may already be registered and have ESs.

<sup>122</sup> A respective project has recently been launched by the Umweltbundesamt “Efficiency of risk management measures for emission reduction” (FKZ 3711 63 419) and is currently performed by Ökopol

The debate on mixture toxicity is of high priority EU level but should be discussed separately from the REACH process of consolidation<sup>123</sup>.

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<sup>123</sup> A project that assesses the feasibility of integrating mixture toxicity aspects in the REACH processes has recently been launched by the Umweltbundesamt to further work on this aspect. "Mixtures in the environment – development of assessment strategies for the European chemicals regulation REACH" (FKZ 3711 63429)

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