

SUMMARY NOTES FROM ECHA WORKSHOP ON SUBSTANCE IDENTIFICATION AND 'SAMENESS' 6 & 7 OCTOBER 2014

PARTICIPATION (SEE LIST):

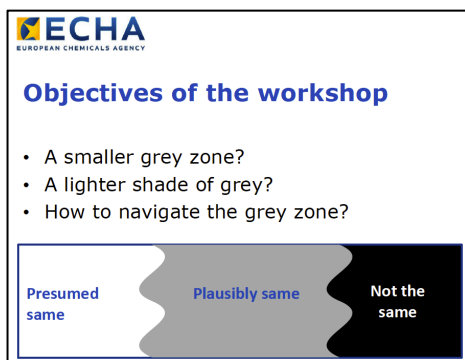
About 30% ECHA, 5% European Commission, 35% Member State Competent Authorities and 30% Stakeholders:

- ECHA:
 - SID & Data Sharing Unit (organiser) and Legal Affairs Unit (C. Jacquet), with occasional attendance by other Units (Derek Knight, Watze De Wolf, Wim De Coen, Bram Versonnen, ...)
 - Opening by Geert Dancet (Executive Director), chaired by Christel Musset (Director of Registration) on 1st Day and by Guilhem De Seze (Director SID) on 2nd day
- European Commission: DG Enterprise, DG ENV, JRC
- Member State Competent Authorities: Finland, France, Germany + other (less active) MSCA (Estonia, Sweden, Denmark, Hungary, Slovak Republic, Latvia, Norway, Portugal, Poland, Lithuania, Austria, The Netherlands)
- Stakeholders: CEFIC (+ companies from various sectors), Eurométaux (Katia Lacasse + Katrien Arijns), Euromines, Concawe, Industrial Minerals association, IFRA, IP consortium, EFEO, LOA, EFR, ECGA

DAY 1 – OPENING AND INTRODUCTION

Geert Dancet opened the workshop reminding participants about the importance of SID for registration's follow up steps. This workshop is already the 3rd ECHA workshop dealing with substance sameness concepts. ECHA has an obligation to support SMEs, in particular in view of the upcoming 2018 registration deadline.

Guilhem De Seze set the scene, outlining challenges ahead and objective of the workshop in addressing the question of "who can register together". Between the "presumed the same" conclusion and the "not the same" conclusion, a "plausibly the same" conclusion exists that participants are requested to address in the workshop.



Cyril Jacquet further reminded the rights and obligations resulting from SID considerations, both from the legal and the scientific aspects. He insisted on the proportionality principle that commends ECHA to not go beyond what is suitable and necessary to achieve the objective of registration, i.e. collect all available and relevant information to assist identifying the hazardous properties of a substance (Recital 17). Although clear SID/sameness is essential, it is not per se the objective of the registration. Therefore **SID/sameness considerations must be made with the aim of identifying the hazardous properties of the composition(s) concerned**. He acknowledged that deviation from established SID rules may be allowed and that registrants may exceptionally refer to the same data set when there is ambiguous/insufficient composition similarity if they provide valid justification (registrant's responsibility!). Legal aspects to be resolved in this case are the extent to which multiple registrants may benefit from the presumption that a data set baseline applies to all, and the nature/level of argumentation required (to ensure a registrant can refer to data set baseline jointly submitted despite variation of its compositions). He insisted that terminology is essential for a common understanding.

DAY 1 – MSCAS' EXPERIENCE ON SID AND SUBSTANCE SAMENESS

Kristof Seubert - German Federal Institute of Occupational Health and Safety (BAUA):

- For well-defined substances, a joint dossier is often submitted on the basis of the CAS nr (e.g. mono-constituent substances with the same main constituent (=same CAS nr) > 80% are considered the same irrespective of their impurity profile). For UVCBs, a decision about a joint dossier requires very detailed considerations about the data set, and this cannot be done on the basis of the CAS/EC nr alone (although this is a good starting point). Industry should consider the question about compliance of the data set **before** a joint dossier project is started (responsible care).
- The ECHA SID guidance states: *"The basic rule is that substances are defined as much as possible by the chemical composition and the identification of the constituents. Only if this is not technically feasible other identifiers should be used, as specified for the various types of UVCB substances."* Main identifiers for UVCBs are related to source, process and to a group of "other main identifiers" (e.g. chromatographic fingerprints). The guidance further states: *"Where the chemical composition of e.g. a complex reaction product or a substance of biological origin is known, substance identification should be identified either as a mono- or multi-constituent substance, as appropriate."*
- There was some discussion on the minimum amount of analysis to be performed for UVCBs, as defining substances by their chemical composition "as much as possible" is subject to interpretation. ECHA referred to the proportionality principle: only if the efforts to define a substance by the chemical composition are too big, you should rely on other identifiers.
- Experiences from SID checks show that SID deficiencies (e.g. CAS number and name inconsistent, inadequate or no analytical data, UVCB vs. multi-constituent substance) make the sameness discussion difficult.
- There are no defined criteria to decide on UVCB vs. multi-constituent substance. The ECHA SID guidance states: *"It is recognized that there will be borderline cases between well defined substances (...) and UVCB substances (...). It is the **responsibility of the registrant** to identify a substance in the most appropriate way."* It is stressed that test requirements for both options remain the same. BAUA strongly recommends that the test substance is defined more precisely, otherwise SID of the test substance is unclear and data sharing problematic.

Upon a question from the audience about the possible validation of the list numbers published by ECHA, ECHA stated that they have no intention to revise the EC inventory (at least not before the 2018 registration deadline). There is however general agreement (from both the industry and ECHA) that this needs further attention/discussion before bringing it to OECD level, as these list numbers should be considered in a regulatory context.

Cécile Michel - French Agency for Food, Environmental and Occupational Health & Safety (ANSES):

- Same CAS nr does not necessarily mean same substance or composition. E.g. a CAS nr can cover various isomers with various stabilities and different impurities, leading to different toxicity.
- ECHA often only compliance checks/challenges the Lead dossier on SID and other registrants are not informed, while the whole SIEF has the responsibility on "sameness". Moreover, there is no emphasis on the need to clarify also SID for the test substance (should be worst case) and its relevance to the registered substance.
- Specific compositions/forms of certain substances have specific properties leading to specific uses. It should be understood that these properties may lead to specific hazards/side-effects.
- It is important to clarify sameness issues **before** substance evaluation, in order to avoid evaluation of a substance for which the registration dossier covers various non-characterised substances and includes data that are potentially not on the relevant substance.
- Strong messages need to be sent to registrants with the technical SID compliance check:
 - SID issues are critical issues that challenge the validity of the registration.
 - When there is an SID issue with one registrant in a joint submission, all registrants in the joint submission should be informed of the potential need for clarification/confirmation that substances are the same.

- There is a need to check that registered and test substances are relevant and appropriate or that relevance/read-across is justified. It is the registrants' responsibility to prove that the data provided by the Lead is applicable to the other composition(s) or form(s).
- There was a call for transparency and a strong call for cooperation: **it is the SIEF's common responsibility to clarify SID.**

DAY 1 – SUBSTANCE SAMENESS – CONCEPTS AND DEVELOPMENTS OF A METHODOLOGY

Ronan Nicolas – ECHA:

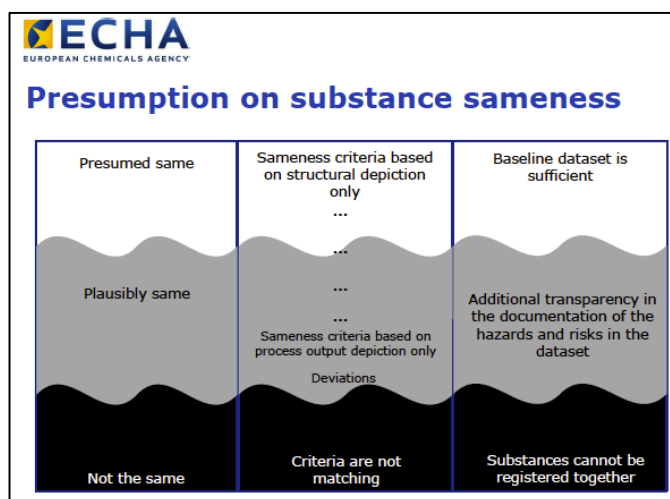
- The presentation addressed the question “what can be registered together?” i.e. what are the SID limits beyond which more than one substance would be covered? It was noted that the SID limits addressed in a registration can evolve over time.
- Substance sameness criteria must not go beyond what is necessary to achieve the objectives of identifying the hazards, assessing the risks and recommending the appropriate RMM for substances.
- A number of substance sameness criteria already exist (e.g. SID of well-defined substances is based on the identity of the main constituents) and should not be re-defined. Moreover, different standards for different substance types (mono-/multi-/UVCB) should be avoided.
- About 15% of the registered substances are UVCBs and it was noted that substance sameness is not a concern for all these UVCBs.
- ECHA guidance imprecisely qualifies when UVCBs are likely to be different: “Any significant change of source or process would be likely to lead to a different substance that would be registered again”.
- The importance of REACH **Recital 45** was stressed: “EINECS included certain complex substances in a single entry. UVCB substances may be registered as a single substance under this Regulation, despite their variable composition, provided that the hazardous properties do not differ significantly and warrant the same classification.” This may be understood in light of the objectives of the registration process:
 - The separate registration of substances is based on the presumption that different hazards and risks will potentially result from different compositions.
 - The variability in the composition of UVCBs is not a reason as such to register substances separately. This does not mean that different UVCBs can be registered together as a single substance.
 - However, establishing sameness based only on the hazard similarities and C&L considerations lacks predictability. In addition, the same substance does not necessarily have the same hazard profile.
- The limits of **EINECS** for SID have been recognised: one EINECS entry may correspond to several substances or several EINECS entries may correspond to one and the same substance. The CARACAL paper on Q&A regarding the role of EINECS (2010) states “In case of doubt, it is recommended to share data as widely as possible [...] and, at the same time, to interpret the substance definition narrowly”. It was stressed that **uncertainties on substance sameness should be resolved regardless of whether a substance is covered by EINECS or not.**
- The proposed tiered approach defines general substance sameness principles for UVCBs, and is based on the EINECS reporting rules (no introduction of new substance sameness criteria):

- 1) Identify the parameter(s), if any, allowing a **structural representation** of the substance
- 2) Identify any additional necessary parameter(s) necessary to represent the substance by the **reaction scheme**
- 3) Identify any additional necessary parameters necessary to represent the substance by the **process**

The combination of above parameters sets the criteria for substance sameness.

- **Structural representation:** starting point is the structural representation of well-defined substances, which is achieved by the “**80% rules**”:
 - 80% rule (mono-): no need to go beyond representing 80% of the composition of a substance.
 - 80-10% rule (multi-): when it is not possible to define 80% of the composition by a unique structural depiction, a structural (qualitative) representation of the composition based on the identity of the main constituents is considered.

- The structural depiction of well-defined substances is normally sufficient to determine if substances can be registered together (same structural depiction -> substances can be registered together; different structural depiction -> substances cannot be registered together).
- Application of the 80% rule to UVCBs should be understood as a means to compare compositions between UVCBs. UVCBs systematically presenting different structural depictions should not be registered together.
- The 80% rule can be seen as a coherent substance sameness criterion applicable across substance types (mono-/multi-/UVCB) and minimises possible discriminations between substance types. However, UVCBs require other types of information for their identification in addition to the composition (composition is only first criterion).
- As an example, a recent case was presented subject to an appeal (A-008-2012 – http://echa.europa.eu/documents/10162/13575/a-008-2012_boa_decision_en.pdf): the application or non-application of a dust extraction step in the process resulted in systematic differences in compositions. In this case, the composition was considered the root cause for differentiating between substances, and two different substances cannot be registered in the same registration dossier regardless of whether they have the same hazard properties.
- **Reaction scheme:** depiction consists of the identity of the reactants and the reaction type.
- **Process:** according to the EINECS reporting rules, the depiction essentially consists of:
 - **Identity of the precursors**
 - **Technology:** definitions of EINECS-listed UVCBs can be used as a reference for the technology depiction. It was stressed that registrants should focus on the parameters that matter for SID!
 - Different process parameters do not necessarily mean that the technology depiction will be different (e.g. reaction t° 100°C vs. 120°C).
 - If the inherent variability does not allow the definition of a technology parameter, such parameter should not be used as a substance sameness criteria (e.g. secondary sources & variability over time).
 - **“Typical” composition:** already taken care of at the level of the structural depiction according to the proposed methodology.
- Outputs from processes relying on different sources or process technologies would in principle not refer to the same substance.
- It was noted that deviations from the proposed methodology are not excluded.



DAY 2 – CHALLENGES FACED BY REGISTRANTS TO ESTABLISH SUBSTANCE SAMENESS

Erwin Annys – CEFIC: Reflections on SID from chemical industry:

- CEFIC published all their REACH documents openly on their website, including a **Substance Identification Profile (SIP)** for mono-constituent substances. A version for multi-constituent substances and for UVCBs is under

development by a consultant and should be available soon. This SIP is a useful tool to establish sameness and hazard data needs. It is usually handled by a trustee.

- CEFIC stressed that ECHA should not change any requirements regarding SID as this may create additional burden. However, clarifications of existing guidance are welcomed in view of the upcoming 2018 registration deadline.
- It is supported that ECHA takes the EINECS reporting rules as a starting point of the proposed methodology, as SID practice has been based on EINECS definitions and experiences. Furthermore, it is appreciated that ECHA recognizes the importance of expert judgement and decisions for non-simple cases (by including a category “Joint registration is plausible, if justifiable”). The general approach for substance sameness should allow the necessary flexibility.
- Reference was again made to Recital 45 (UVCBs may be registered together despite their variable composition, provided they have the same classification), which is not in line with the CLP Regulation (different classifications for the same UVCB are possible).
- CEFIC sees no legal mandate for restrictions by the 80% rules for UVCBs.

Paula Karjalainen – CEFIC (Nesteoil): Hydrocarbon (HC) solvents:

- HC solvents are usually UVCBs, but may also be mono- or multi-constituent substances. Their complexity mainly comes from the increasing number of isomers with increasing carbon number.
- Prior to REACH registration, there was no common naming system for HC solvents. EINECS descriptions existed for a number of HC substances but these were too broad according to REACH needs and sometimes several EINECS numbers existed for one HC substance. Therefore, a **naming convention** was developed based on the ECHA SID guidance. Products of similar composition and similar use should be the same substance and one HC solvent should have one classification to the extent possible.
- For UVCB HC solvents, the name consists of 1) "Hydrocarbons", 2) the C number range (including $\geq 80\%$ of the components of the substance), 3) the description of the HC structures present (n-paraffins / isoparaffins / naphthenes / aromatics), and 4) components with specific toxicology or classification (using the classification cut-off as an indication level).
- “**Same** substances” fall within the compositional parameters defined by the naming convention.
- “**Similar** substances” are grouped into categories for hazard characterization. A chemical category is a group of chemicals whose phys-chem and toxicological properties are likely to be similar or to follow a regular pattern as a result of structural similarity. HC solvent categories were based on common constituents with similar C numbers. The differentiating characteristics are C number range, aromatic content, and the presence of n-hexane and/or naphthalene at toxicologically relevant levels. Because the category members have structural similarities, there are predictable patterns in phys-chem properties, resulting in similarities in human and environmental health effects and environmental fate properties. Thus, hazards for substances in each category can be characterized on a generic basis using data from studies of representative substances.

Stephen Harley – Concawe: Specific features of petroleum UVCB substances:

- Petroleum substances are UVCBs arising from many refinery processes. Their SID is based on EC descriptions. **Existing EC inventory entries** are preferred rather than inventing multiple new substance ID's. The Concawe guidance is consistent with the ECHA SID guidance.
- Petroleum substances are described by C number range / boiling point range / process. These parameters give an indication of the chemical composition, which is complex and variable. The number of individual chemical compounds increases rapidly with increasing C number.
- Stream composition varies continuously over time due to feedstock composition, processing severity, separation temperatures, sharpness and catalyst / equipment performance.
- For the manufacturing process, there may be slight differences between registrants, but the Concawe approach is to follow the established EINECS level of detail and avoid excessive detail.

- Concawe uses a **category approach** to avoid underestimating the hazard. Substances of similar composition are grouped based on process history and C number / boiling point range. Per endpoint, value or hazard driver(s) are identified. Data gaps are filled in by read-across from worst case to ensure proper risk management. Category outliers are identified based on C number / boiling point range / hydrocarbon classes.
- To correctly and practically consider the hazards, **testing is conducted on the whole substances**, not individual constituents or groups of constituents.
- There is a programme ongoing to gather more analytical data to verify SID. There is no universal set of methods for all the petroleum substances. Concawe will analyse samples of each registered substance with both standardized and advanced techniques, including identification of constituents expected to drive hazards. Concawe recommends registrants to continue analysing their substances with standardized techniques. If standardized results are within the Concawe-reported ranges and the manufacturing process applies, it can reasonably be assumed that detailed composition is within the range covered by the Concawe category.
- Concawe noted that the **80% rule** is difficult to apply as such to petroleum substances: EC descriptions for petroleum substances often use the terms “predominantly” and “approximately” instead of quantitative limits. However, these qualitative limits may be sufficient for sameness purposes and to ensure that the reported composition fits the description.

Katia Lacasse – Eurométaux: Inorganic UVCBs:

- Inorganic UVCBs are complex materials that contain varying concentrations of metals, metal compounds and/or minerals (often composed of 10 or more constituents). They result from the refining of primary and/or secondary **sources**, i.e. complex materials with an intrinsically variable composition, leading to variability in composition of the resulting UVCB. Furthermore, this variety of variable sources is often fed simultaneously or sequentially to the production process and sources are not always processed separately. Therefore, sameness of inorganic UVCBs is mainly based on processes used.
- Generally, common **processes** are used across the sector and the starting point to describe these processes was always the commonalities. When there were slight differences in processes between registrants, it was checked if these differences imply different registrations (e.g. by testing). Expert judgement was used to select the most appropriate material to test for SID refinement purposes. Where possible, the NFM BREF was used to describe processes. Generic process flows were produced to identify the occurrence of different UVCBs.
- Fitting **EINECS entries** were originally identified on the basis of the name or description of the EINECS entry, which was not always 100% consistent with the ECHA SID Guidance but either already used as identifier for the material or sufficiently similar to be used for registration purposes following the original SID and sameness assessment. Improvements of EINECS descriptions were suggested where necessary, consistent with the ECHA SID guidance. For those substances where there was no EINECS entry, new substance ID's were created.
- Overlap with other consortia's scopes were identified and discussed as needed.
- Information on company specific **compositions** (elemental + speciation) was exchanged with the consortium secretariat, on a confidentiality basis. The secretariat then developed a “generic” composition across industry. The temporal variability in composition for a specific registrant is assumed to be covered by the across-registrant variability.
- The variability in composition of inorganic UVCBs can lead to different **hazard** profiles: 1 UVCB can have several (classification) grades. Periodic re-assessment of classifications/hazard profiles is necessary.
- The SID profile / ID card and common testing protocol are basis for evaluation (“reasonable” level of details to be agreed upfront).
- It was noted that the **80% rule** is difficult to apply as such to inorganic UVCBs as this is very restrictive. For inorganic UVCBs, the decision on sameness is not solely made based on the composition!

DAY 2 – BREAK OUT GROUPS AND CONCLUSIONS

1) Petroleum substances

2) Hydrocarbon solvents

3) Metals

- Based on the composition of the provided example (a Cu matte), there was discussion on whether the substance could be considered a multi-constituent substance. The variability of inorganic UVCBs was stressed. ECHA stressed that the choice UVCB versus multi-constituent substance does not lessen the obligation to provide information.
- The importance of providing speciation information in the composition was stressed.
- There was general agreement that additional parameters are needed for SID in addition to the composition. If you only take composition into account, the substance could be regarded a mixture. Process information is also important to identify the substance.
- There was discussion on which constituents to take into account for SID. Only those present > 10%? Only those with a classification? The constituent definition needs to be aligned.
- ECHA stressed the need to ensure transparency of SID in the registration dossier.
- It was noted that ECHA should clarify that structural depiction of the substance refers to the chemical structure.

4) Organic dyes

DAY 2 – WRAP-UP AND CONCLUSION

- Both the different industry sectors and the MSCA are still struggling with SID of UVCBs.
- There was general support to explore the applicability of the proposed 3-step sameness methodology (structural representation/reaction scheme/process output) further, but there were still quite some questions on how it will work in practice. ECHA does not have all the answers to these questions and recognises there will always be a “grey zone” for SID of UVCBs.
- In the “grey zone”, after using the proposed methodology, it is important to make the argumentation that the chosen SID approach is sound.
- The use of hazard information in deciding on SID of UVCBs requires further discussion. There was general agreement that different classifications can be covered in a joint registration.
- Informal feedback from the metals break-out session indicated that ECHA does not expect us to revise our SID approach completely but thinks **some further work is needed from industry's side to rationalise and document our SID approach so that it is transparent.**
- The proceedings from the workshop will be published on ECHA's website. ECHA agreed that workshop documents can be shared.

FROM THE CARACAL DOCS

In a nutshell, the founding principles of the proposed methodology are based on the general rules applied for reporting UVCB substances in EINECS. These rules relied on as precise as possible depiction of UVCB substances using essentially any of the three possible types of representation (structural representation; reaction scheme; process description) or any combination thereof. The methodology takes also into account the regulatory knowledge acquired on substance sameness under Directive 67/548/EEC and REACH. The result is a structured approach enabling substance sameness criteria to be defined. **The combination of these criteria should provide a depiction, to the extent possible, of what a substance consists of.** The developed methodology therefore sets **priority to the structural representation** followed by the reaction scheme and the process output. **This hierarchy requires considerations on the description of the composition to be made first** before any other additional depiction is applied to define the substance sameness criteria.

The methodology recognises the limits of identifying UVCB substances by their chemical composition. Accordingly, it does not require setting substance sameness criteria based on the structural representation only. It entails instead the identification of systematic structural characteristic which, if the substances were to be well-defined, would constitute substance sameness criteria. The structural depiction therefore relies on the “80% rules” established for well-defined substances.

Another important aspect of any proposal on substance sameness is that it should **not go beyond what is necessary to meet the objectives of the registration process.** The proposed methodology allows registrants to deviate from the rules for setting the substance sameness criteria, as it can be done for well-defined substances. The deviation must however be clearly and transparently justified. These permissible deviations provide the flexibility needed in the practical implementation of the registration process.

This methodology should overall be seen as a prolongation of existing substance identification principles and therefore not in contradiction with the Guidance on substance identification.