

Substance sameness – concepts and development of a methodology

SID workshop

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Sharing
European Chemicals Agency



OUTLINE

1. Important considerations
2. Substance sameness – the facts
3. Link between EINECS and substance sameness
4. Proposed approach
5. Conclusions



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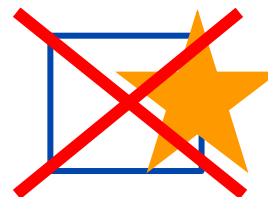
Important considerations (1/3)

- Behind the terminology “substance sameness” is the key question “what can be registered together?”
- “What can be registered together?” and “what is registered together?” are different questions
 - “What can be registered together?” = what are the SID limits beyond which more than one substance would be covered?
 - “What is registered together?” = what are the SID limits addressed in a registration dossier?

**This presentation addresses the question
“what can be registered together?”**

Important considerations (2/3)

- The SID limits addressed in a registration must fit within the SID limits for one substance



- The SID limits addressed in a registration may be smaller than the SID limits for one substance



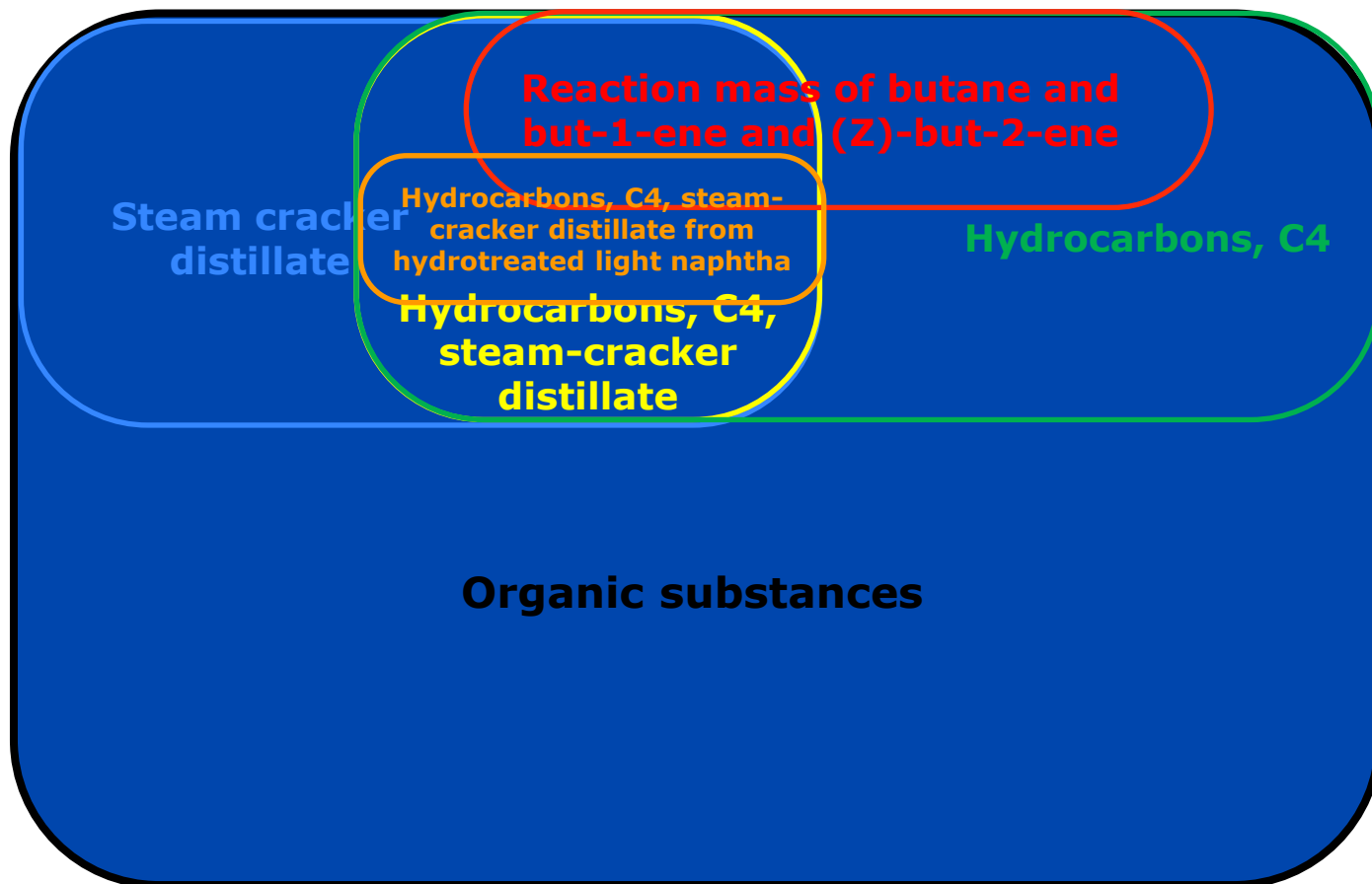
- The SID limits addressed in a registration can evolve over time



Important considerations (3/3)

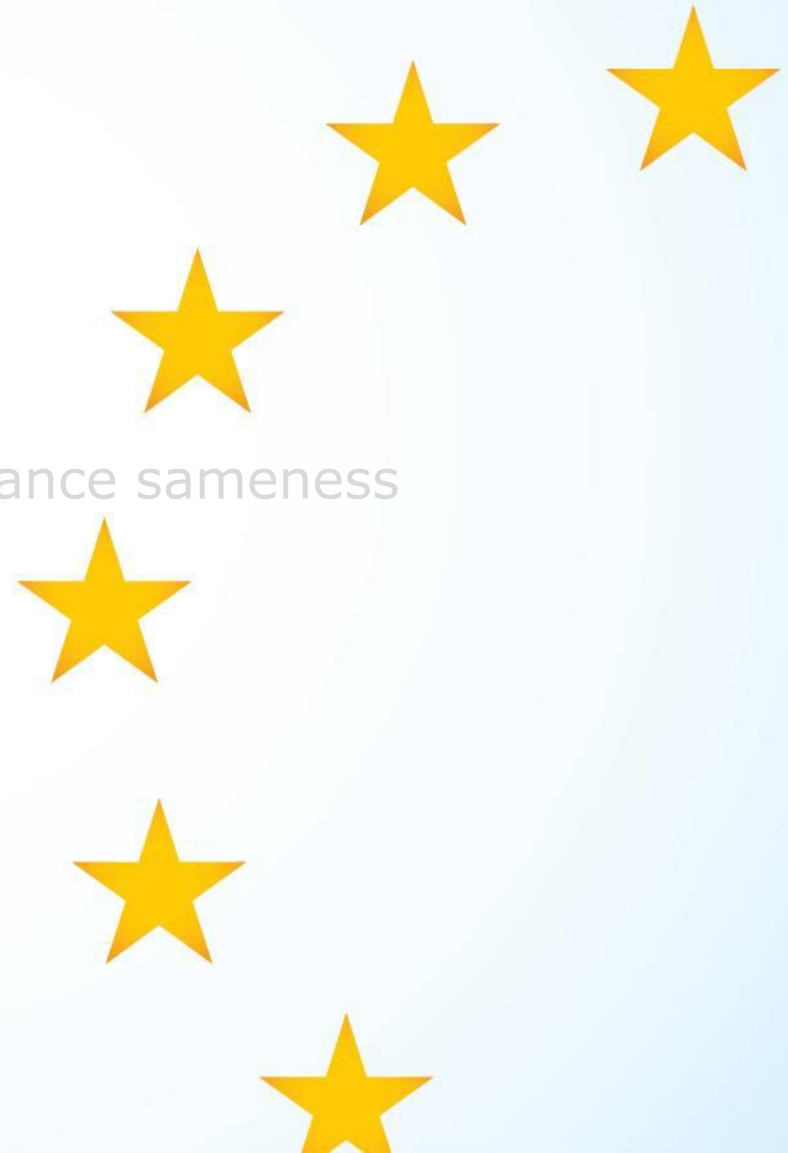
- Substance sameness criteria under the Registration process must be proportionate to the objectives of identifying the hazards, assessing the risks and recommending the appropriate RMM for substances
- Substance sameness criteria exist
 - Substance sameness principles in REACH and the Guidance should be followed
 - Well-established criteria should not be re-defined!
- Substance sameness criteria must be overall coherent
 - Discriminations between substance types (mono-/multi-/UVCB) should be avoided
- Established exceptions/derogations should not dictate the general substance sameness principles

An illustration of the task – where to set the SID limits



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Substance sameness – the facts

- EC inventory provides a mapping for a significant number of substances concerned by the registration process
- A number of substance sameness criteria are secured in the Guidance
 - Representation of well-defined substances based on the identity of the main constituents
 - The same substance does not necessarily have one unique “hazard” profile
 - Deviations allowing substances normally considered different to be regarded the same (justifications based on hazard data, C&L, uses)
 - Limited set of qualitative criteria when 2 UVCB substances cannot be regarded the same
- Recital 45

Registered substances – measuring the level of certainty on substance sameness

- 85% well-defined vs. 15% UVCB substances
- Limited concerns for well-defined substances
- Not a concern with all UVCB substances

What makes substance sameness between UVCB substances so complex? (1/2)

- Complex substances
- The EC inventory does not always provide a coherent mapping of UVCB substances
- The Guidance imprecisely qualifies when UVCB substances 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”

What makes substance sameness between UVCB substances so complex? (2/2)

- Recital 45 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 UVCB substances is not a reason as such to register substances separately
 - This does not mean that different UVCB substances can be registered together as a single substance
- However...
 - Establishing sameness based only on the hazard similarities and C&L considerations lacks predictability
 - The same substance does not necessarily have the same hazard profile

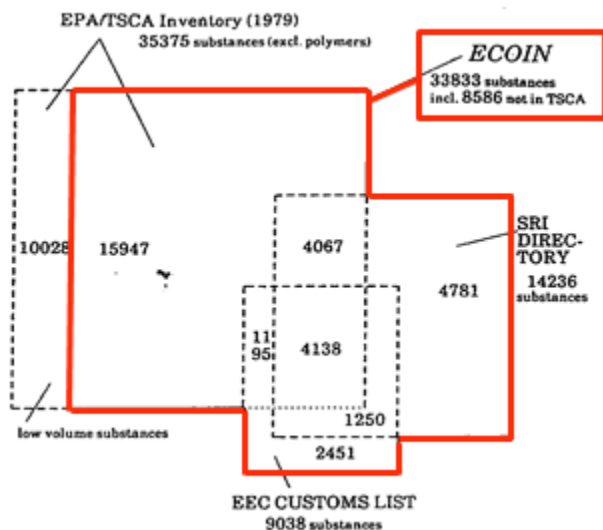
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EINECS is a compilation of inventories

- EINECS = ECOIN + reported entries from a pre-defined "compendium" + other substances reported for EINECS



Compendium of known substances

(>28000 entries)

Substances reported using

- form B (substances listed in CAS)*
- form C (substances without CAS#)*

Reporting rules and EINECS compilation

- The EINECS reporting rules were tailored to accommodate foreseen discrepancies on the identification of substances

18 Special categories have been established and included in ECOIN covering all of the component substances intentionally produced in certain common commercial reaction mixtures.

Examples:

Cement, Portland, chemicals [65997-15-1 *]

Cement, alumina, chemicals [65997-16-2*]

Glass, oxides [65997-17-3*]

Frits, chemicals [6.997-18-4*]

Ceramic materials and wares, chemicals [66402-68-4*]

Steel manufacture, chemicals [65997-19-5*]

Definitions for these examples can be found in the "Chemical Substance Definitions Section" of ECOIN. Only substances or categories not fitting those included in ECOIN can be reported.

- Discrepancies in EINECS were unavoidable
- The discrepancies did not compromise the use of EINECS under Directive 67/548/EEC

UVCB substances – EINECS inconsistencies

- EINECS was not required to consist of a list of single substances
- The limits of EINECS for the identification of substances covered by the inventory has been recognised

Guidance on substance identification

“It is important to note that for some EINECS entries, the description of a substance is relatively broad and could potentially be considered to cover more than one substance”

CARACAL paper on Q&A regarding the role of EINECS (2010)

“One EINECS entry may also correspond to several substances or several EINECS entries may correspond to one and the same substance”

“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”

- Recital 45 indicates that multiples substances may be covered by the same EINECS entry
- Uncertainties on substance sameness still to be resolved regardless of whether a substance is covered by EINECS or not!

EINECS inconsistencies - example

- EC# 269-816-4 for “Fatty acids, tall-oil, triesters with sorbitol”
- EC# 294-984-0 for “Fatty acids, linseed-oil, monoesters with sorbitol”
- EC# 294-316-8 for “Fatty acids, peanut-oil, esters with sorbitol”
 - Is the substance consisting of 100% sorbitol triesters of peanut-oil fatty acids covered by the EINECS entry?

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How to look at the proposed approach

- The proposed approach defines general substance sameness principles for UVCB substances
- Keep in mind that the principles should be applicable to any substance, including phase-in and non-phase-in substances
- Look at the proposal from a distance before considering how the proposal would apply to a specific substance

Substance sameness criteria- Proposed approach

- The consistent element in the identification of UVCB substances for EINECS stands at the level of the EINECS reporting rules (form C – substances without CAS#)
- Start from the principle that these EINECS reporting rules are sufficient as a baseline to establish substance sameness
- Harmonise the rules with the definite substance sameness principles established over time
- No introduction of new substance sameness criteria

EINECS reporting rules for UVCBs (1/2)

- Six methods for depicting UVCBs:
 1. Structural representation
 2. Reaction scheme
 - Identity of the immediate precursors
 - Identity of the reactants
 - Reaction type
 3. Process description
 - Precursors
 - Technology (method of preparation; process terms)
 - Typical composition
 4. Genus and species specifications
 5. Combination of the abovementioned methods
 6. Conventions for the identification of soap and detergents

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EINECS reporting rules for UVCBs (2/2)

- One guiding principle for EINECS reporting: the substance, its constituents or precursors should be specified as precisely as possible
- Towards ranking of the rules for depicting UVCBs according to a structured approach
 - Structural representation
 - Reaction scheme
 - Process description
- Separate conventions should be defined for each method of depiction

Proposed substance sameness criteria

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

The combination of these parameters set the criteria for substance sameness

A simple illustrative example

- Case of a substance resulting from the full esterification of coco fatty acids with trimethylolpropane

- 1) Structural representation: triesters
- 2) Reaction scheme representation: reaction products of coco fatty acids with trimethylolpropane
- 3) Process representation: not required

Substance sameness criteria: the same substance needs to refer to triesters and to correspond to reaction products between coco fatty acids and trimethylolpropane

Structural representation

- Starting point: structural representation of well-defined substances
 - 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

80% rules across substance types

- Not a new concept for UVCB substances!
 - NLP list: “Mixture of oligomers or isomer mixtures are generally listed in the no-longer polymer list with the name of the main component only when present in the mixture with 80% or more”
- A principle considered relevant when defining coherent substance sameness criteria across substance types
 - Avoid discriminations between substance types
 - As a baseline, a criterion preventing substances from being registered together would apply regardless of the substance type

Application of the 80% rules to UVCBs (1/2)

- The use of the “80% rules” for depicting the composition of UVCBs is not about requiring UVCBs to be identified as well-defined substances
 - The composition is normally not sufficient to identify UVCB substances
 - UVCB substances require other types of information for their identification, in addition to what is known about their composition

Application of the 80% rules to UVCBs (2/2)

- The application of the rules should be understood as a means to compare compositions between UVCBs
- UVCB characteristics (unknown/variable/complex composition) must be taken into account in the structural representation
 - Focus on structural characteristics of the constituents in the substance
 - Substances systematically presenting different structural depictions would normally not be registered together

UVCB structural depiction - Examples (1/3)

- A substance X consisting of $\geq 80\%$ of diesters of “UVCB reactant A” and “UVCB reactant B” can be depicted structurally as “diesters”
- A substance Y consisting of $\geq 80\%$ of triesters of “UVCB reactant A” and “UVCB reactant B” can be depicted structurally as “triesters”
- The difference in the structural depiction between substance X and substance Y would be a criteria for not registering them together

UVCB structural depiction - Examples (2/2)

- The opportunity of establishing substance sameness criteria based on structural depiction is not limited to “well-defined” UVCB substances
 - Recent case subject to an appeal (A-008-2012))
 - A registration covered substances obtained from different manufacturing processes (application or non-application of a dust extraction step).
 - Systematic differences in the compositions resulted from this difference in the process (either high or very low concentration level of ash constituents in the substances)
 - Composition as the root cause for differentiating between substances
 - Two different substances cannot be registered in the same registration dossier regardless of whether they have the same hazard properties

UVCB structural depiction - Examples (3/3)

- Opportunity in the structural depiction of petroleum substances?
 - The definition of EINECS listed petroleum substances includes structural characteristics
 - Predominantly consisting of/large proportion of...
 - ...aliphatics, alicyclics, branched hydrocarbons, aromatics, tricyclic aromatics, saturated straight chains, 3-membered ring aromatic hydrocarbons...
 - ...in the range of C_x through C_y
 - Reference to the 80% rules in the COM publication “The EINECS inventory of existing chemical substances on the market” (Toxicol. Environ. Chem., vol.37, 21-33)

4 Petroleum and Coal products

There were requests to give for each reported product as such an EINECS entry of its own, no matter whether these products would overlap. This concept was in conflict with the idea of grouping them into typical products taking into consideration the carbon ranges, boiling ranges, the typical chemical composition and the starting material. The latter concept was finally adopted (giving assurance that entries for larger fractions would cover both smaller fractions and those being incongruent by not more than 20%),

UVCB depiction by the reaction scheme

- The depiction consists of
 - Identity of the reactants as substance sameness criteria
 - “Reaction products of A and B” to be regarded as a different substance than the “reaction products of A and C”
 - Reaction type
- Ratio of reactants is not necessarily a criteria in the proposed approach:
 - Criteria indirectly addressed at the level of the structural depiction
 - No definite borderline between substances according to this parameter (e.g. borderline between substances obtained from reacting A and B where A:B ratio varies from 1:1 to 1:5)
- Examples of reactants ratio in the EC inventory:
 - EC# 291-322-2: Formaldehyde, reaction products with oleylamine and phenol
 - EC# 430-930-6: Reaction product of diphenylmethanediisocyanate, octylamine and oleylamine (molar ratio 1:1.86:0.14)

UVCB substance depicted as the output of a process

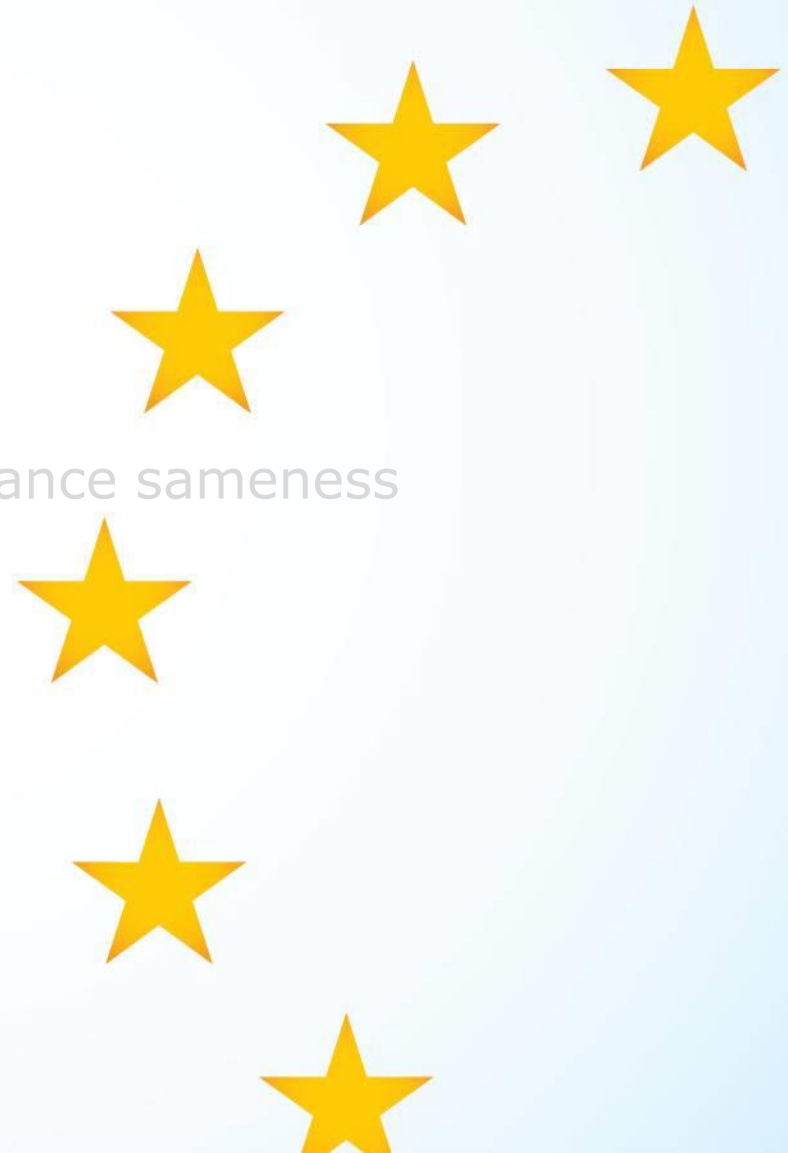
- According to the EINECS reporting rules, the depiction essentially consists of
 - Identity of the precursors
 - Technology
 - ‘typical’ composition
- Outputs from processes relying on different sources or process technologies would in principle not refer to the same substance
- ‘Typical’ composition is taken care of at the level of the structural depiction according to the proposed methodology

Note on the depiction of the technology

- The depiction must be proportionate
 - Different process parameters (e.g. reaction temperature 100°C vs. 120°C, pressure) do not necessarily mean that the technology depiction will be different
 - If the inherent variability does not allow the definition of a technology parameter, such parameter should not be used as a substance sameness criteria
 - Example: identity of secondary sources
- Focus on the parameters that matter!
- Definitions of EINECS-listed UVCB substances as a reference for the technology depiction

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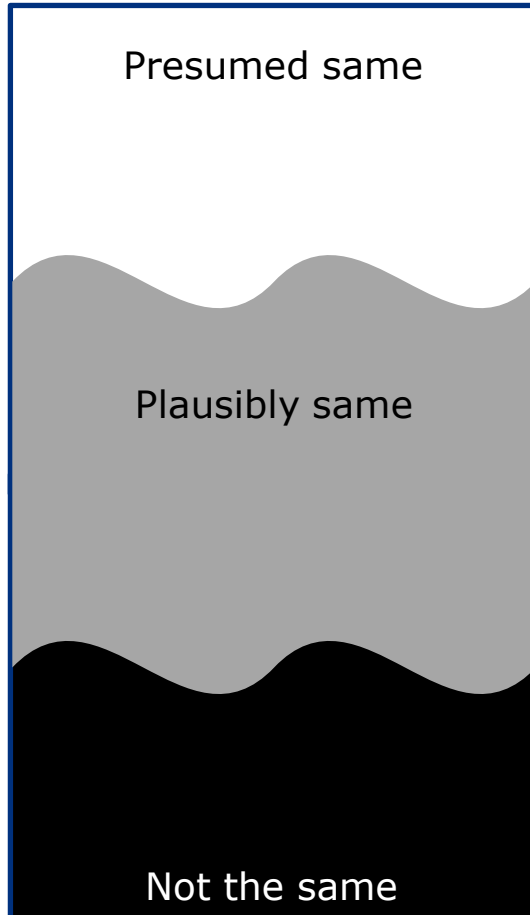
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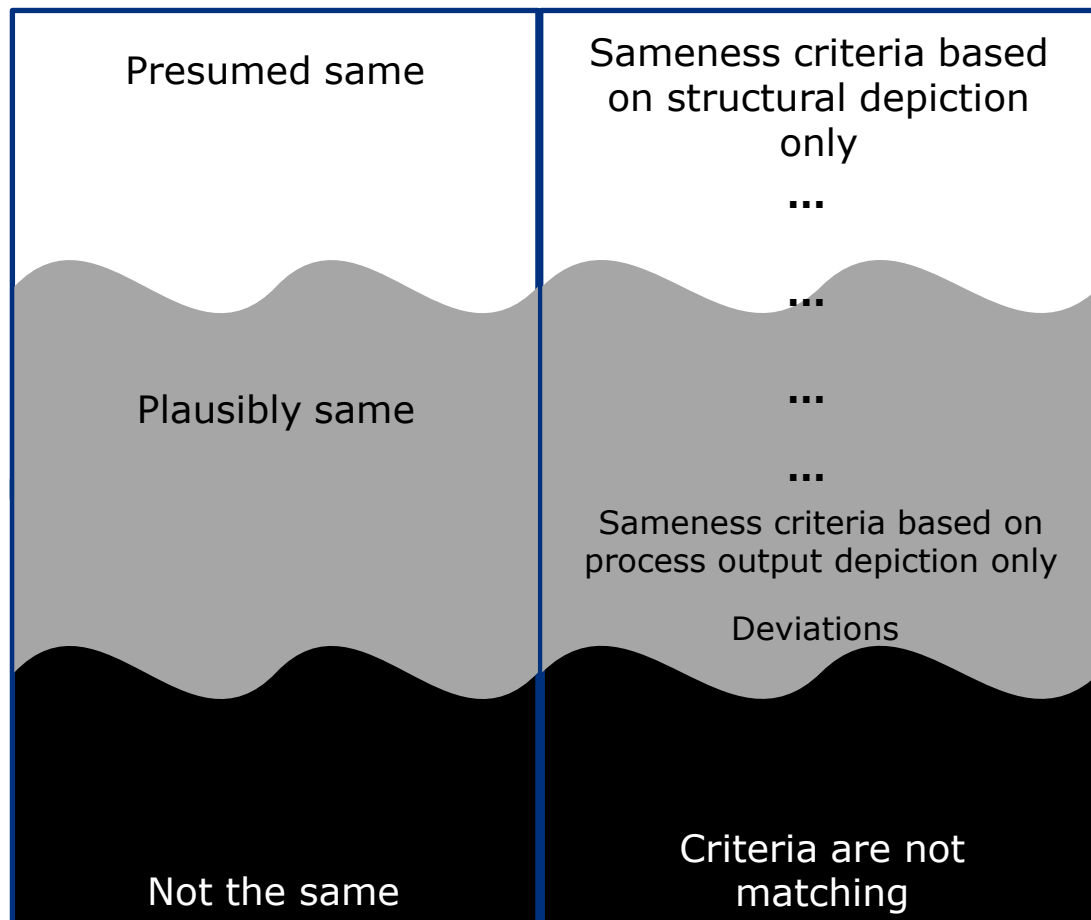
Opportunities of the proposed approach

- Establishes a structured methodology on how to approach substance sameness
- Proportionality of the substance sameness criteria which give priority to the composition
- Minimises possible discriminations between substance types
- Preserve as far as possible the coherent part of the mapping of substances in EINECS
- Minimises the risks of establishing rules that are 'out of phase' with EINECS
- Deviations are not excluded

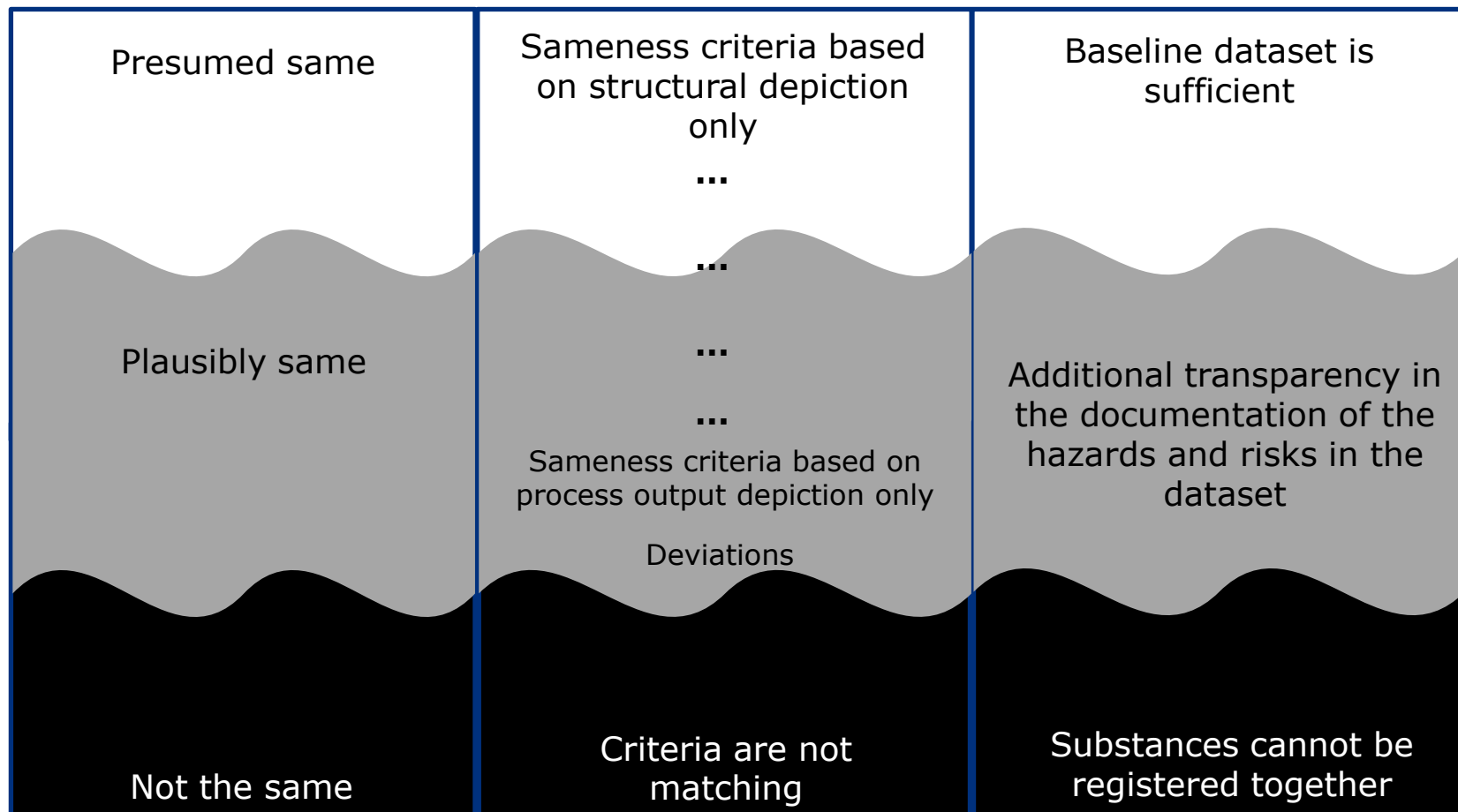
Presumption on substance sameness



Presumption on substance sameness



Presumption on substance sameness



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