# Substance identity - Feedback from ECHA

## REACH Information and Experience Exchange Forum (RIEF I)

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# Outline of the presentation

- Introduction
  - Importance of substance identification
  - Quality of substance identity information in inquiry and registration dossiers
- General tips to improve dossier SID information quality
- UVCB substances and SID
  - Background
  - Common SID challenges for UVCBs
- Tools and further resources
- Key messages

# Why is substance identity important?

- Chemical identity of the substance is clear
  - What is the substance (to be) registered?
  - Which substances are the same?
  - Who has to register jointly?

- Objectives
  - Joint registration covers one substance
  - Data sharing is efficient and unnecessary testing is avoided
  - Substance identity is clearly defined for hazard and risk communication

# Substance identity requirements

- Substance identity requirements are specified in Annex VI Section 2 of the REACH Regulation

  - *For each substance, the information given in this section shall be sufficient to enable each substance to be identified. If it is not technically possible or it does not appear scientifically necesssary to give information on one or more of the items below, the reasons shall be clearly stated.*

# Quality of SID information in dossiers

- Inquiry
  - 2013: 848 inquiries received by end of May; ca. 1/3 rejected because of missing/inconsistent SID information
- Evaluation
  - SID in registration dossiers with testing proposals
    - 557 dossiers with TP submitted for the 2010 deadline
      → 128 SID tCCH
  - Recommendations for improving SID quality in registration dossiers are available in the evaluation report for 2012
    http://echa.europa.eu/documents/10162/13628/evaluation_report_2012_en.pdf
- ECHA has tools available for automatic screening of registration dossier SID information – screening to be done end of 2013
  http://echa.europa.eu/view-article/-/journal_content/title/e-news-24-april-2013

# General SID recommendations (1)

- Dossier specific for one substance
  - Generic/too broad EC/CAS identifiers should not be used for specific substances
- Information in the dossier specific for your substance as manufactured
  - Manufacturing process (UVCB substances)
  - Composition: constituents and concentrations
  - Analytical information recorded on your substance
- Avoid industry specific abbreviations, trade names, etc.

# General SID recommendations (2)

- Ensure that the information is sufficient
  - All required information specified in Annex VI(2) is provided, including analytical information
  - The information provided is sufficiently detailed, including descriptions for analytical methods
  - If the general requirements are not applicable to your substance or if they are not sufficient
    - include additional information, e.g. analytical results from other methods (e.g. XRD for inorganic substances), and
    - include robust and scientific justification if not including a general information requirement; ”I don’t have an IR” or ”it does not provide more information” are not sufficient justifications ☺

# General SID recommendations (3)

- Ensure that the information provided is consistent
  - Provided identifiers refer to the same substance
  - Identifiers match with the composition
  - Compositional information matches with the substance you manufacture and is sufficiently detailed; grades reported separately
  - Analytical information is in line with the identity the and composition

# UVCB substances and SID

# UVCB substances

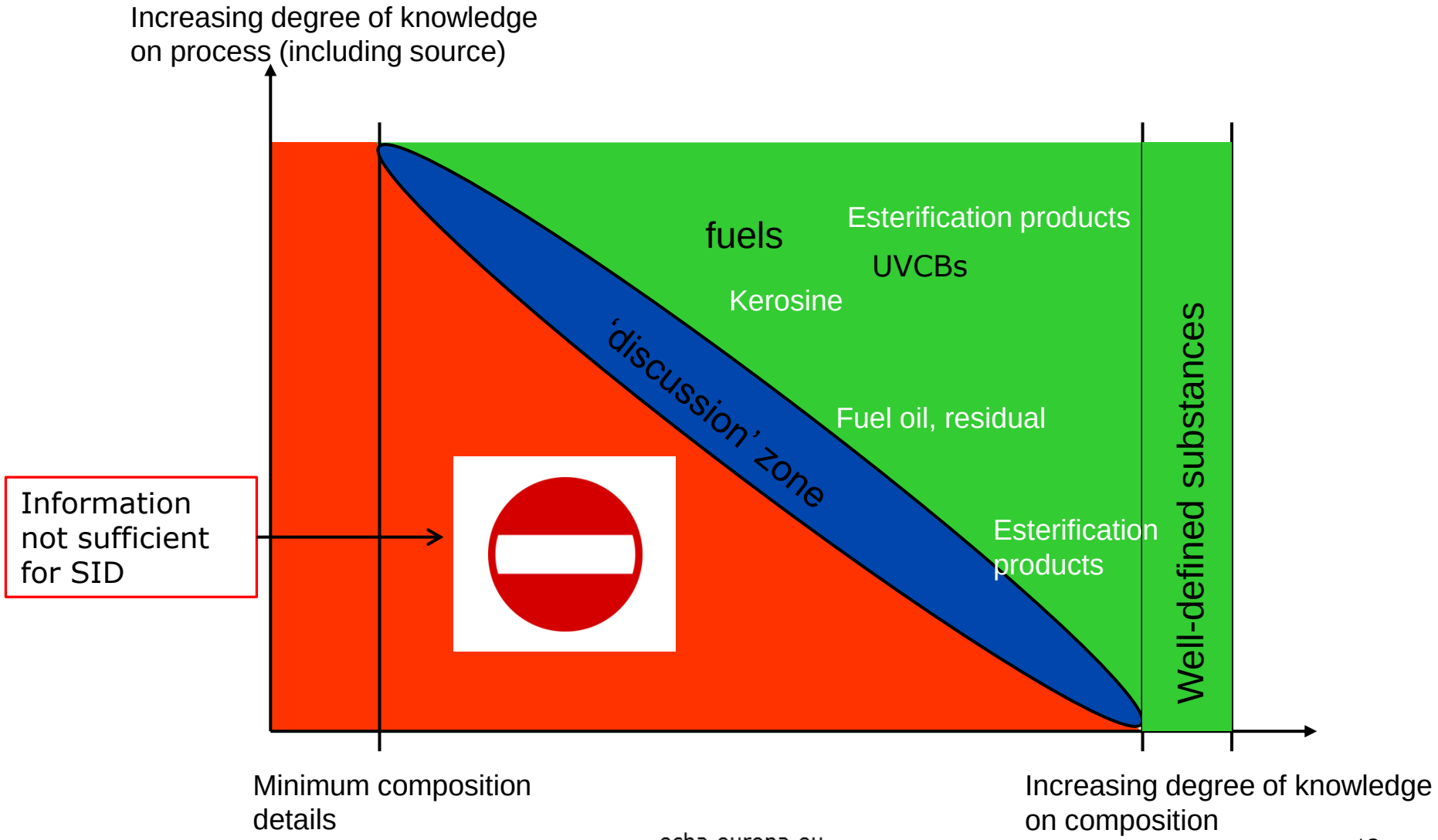
- Substances of:
  - **U**nknown or **V**ariable composition,
  - **C**omplex reaction products or
  - **B**iological material
- Cannot be sufficiently identified by chemical composition
  - The number of constituents is relatively large and/or
  - The composition is to a significant part unknown and/or
  - The variability of composition is relatively large or poorly predictable
- UVCB substances require other types of information for their identification, in addition to what is known about their chemical composition

# UVCB substances

- Main identifiers for various types of UVCB substances are related to:
  - Source of the substance and
  - Process used for obtaining the substance (e.g. reaction type).
- Significant change of source or process would lead to a different substance.

- The requirements for substance identification as described in Annex VI (2) to REACH apply also to UVCB substances. Analytical information has to be provided.

# Why is manufacturing process important?



# Common SID challenges for UVCBs – manufacturing process

- Manufacturing process needs to include information on:
  - starting materials and their ratios
  - reaction type(s) (e.g. esterification, alkylation…)
  - processing steps (e.g. reaction, extraction, distillation…),
  - processing parameters (e.g. temperature and pressure)
- If EINECS includes a description of the substance ensure that the provided process description/information on constituents is in line with this information

# Common SID challenges for UVCBs - composition

- Not enough to describe the composition as ”100% my substance”
- Composition needs to include
  - known constituents irrespective of their concentration
  - constituents/groups of constituents in line with the chemical species in the substance identified as far as possible;
    generic groups of constituents can be reported (e.g. linear alkanes C7-C12, mono-aromatic hydrocarbons)
  - typical concentrations and realistic concentration ranges specific for your substance
- If several grades are covered, it is recommended to report the grades as different composition blocks instead of one generic composition

# Common SID challenges for UVCBs – analytical information

- General REACH requirements of Annex VI(2) for analytical information apply also to UVCB substances – if something is not included justification needs to be added
- Included analytical information needs to be sufficient to identify and quantify the constituents included in section 1.2
  - Any additional information that is necessary to demonstrate this is recommended to be included (e.g. other analytical methods, reaction mechanisms, theoretical calculations…)

# UVCB examples – manufacturing process

1. An aqueous solution (…%) of A is acidified by addition of acid X in a 1:1 molar ratio to form B at temperature $T_1$.
2. This solution is then reacted with C, which is dissolved in solvent Y, in a 1:2 molar ratio.
3. This 2-phase reaction forms the substance D, dissolved in solvent Y.
4. The aqueous layer is separated and disposed of.
5. The substance D is purified by distillation at pressure $p_1$ and temperature range $T_2$-$T_3$.

# UVCB examples – composition

- A hydrocarbon-based UVCB substance has been analysed and contains > 50 constituents of which none are > 10 % in the chromatogram. The company has generically presented the composition as follows:
  - Linear alkanes (C20-C32) 60-80 % w/w
  - Branched alkanes (C20-C25) 20-35 w/w
  - Cyclic alkanes (C20-C25) 0-5 % w/w

# UVCB examples – waiving of spectral data

- A company produces a crystalline inorganic UVCB substance.
- The company considers that the list of spectral data in Annex VI 2.3.5 is not the best way to identify the substance but instead applies elemental analysis (XRF) as well as XRD and IR spectral analyses.
- These analyses characterise the substance.
- In addition the company waives NMR and UV spectral analysis based on the substance structure and the fact that more appropriate techniques have been applied instead.

# Tools and further resources

- IUCLID tools
  - Technical completeness check plug-in
  - Dossier quality assistant: TCC plug-in 5.4.3 containing the Dossier Quality Assistant was released on 11/02/2013 – addresses shortcomings in SID
    - Recommended to be used to identify SID deficiencies before ECHA carries out automatic screening (end of 2013)
- Resources on the ECHA webpages
  - Guidance documents
  - Q&A documents
  - Data submission manuals
  - Webinars on SID
  - List available at the end of the presentation

# Key messages

- Correct substance identification is the first step in all REACH processes
- Ensure that the information in your dossier is
  - Specific for your substance
  - Complete regarding the information requirements
  - Sufficient to identify your substance
  - Clear and consistent
- Check your dossier in advance with the available tools
- Visit the ECHA webpages for more information

# Where to find more information

- ECHA substance identity webpage http://echa.europa.eu/regulations/reach/substance-identity
- ECHA inquiry webpage http://echa.europa.eu/regulations/reach/substance-registration/inquiry
- Guidance for identification and naming of substances under REACH and CLP http://echa.europa.eu/documents/10162/13643/substance_id_en.pdf
- Questions and answers on substance identification http://echa.europa.eu/documents/10162/13648/qa_substance_id_en.pdf
- Questions and answers on inquiry http://echa.europa.eu/documents/10162/13652/qa_inquiry_en.pdf
- Data Submission Manual Part 18 – How to report the substance identity in IUCLID 5 for registration under REACH http://echa.europa.eu/documents/10162/13653/substance_id_report_iuclid_en.pdf
- Webinars on SID
  - Importance of substance identification and sharing of data for the 2013 registration deadline - http://echa.europa.eu/view-article/-/journal_content/63e12fa5-cd2e-459e-9925-be7a676a81d3
  - Inquiry process – http://echa.europa.eu/web/guest/view-article/-/journal_content/d660dd16-630a-4c3a-8552-812de10dc616
- TCC plug-in and dossier quality assistant http://echa.europa.eu/view-article/-/journal_content/title/new-tool-to-support-registrants-in-improving-dossier-quality-now-available

# Thank you!

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