

## Chesar training Box 1



17 May 2011



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## Chesar Box 1

- Chesar and IUCLID
- Substance properties in Chesar
- Scope of exposure assessment



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## Chesar Box 1



1. **Manage substances**
2. Reporting of uses
3. Manage assessment
  1. Workers (consumers)
  2. Environment
4. ES building and CSR generation
5. Generation of ES for eSDS
6. Administration tools



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## Overview of BOX 1

- Ensure the **synchronisation** with IUCLID 5 data used in Chesar for assessment
- Trigger an appropriate **scope for the assessment** based on hazards (= type of adverse effect, route of human exposure, affected environmental protection target) identified in the hazard assessment:
  - Classified hazards (CnL)
  - Other adverse effects
- **Manage** all the substances for which an assessment is being carried out or has been carried out with Chesar



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## Chesar and IUCLID 5

- Chesar is a IUCLID 5 plugin
- All information on the **intrinsic properties** of the substance is imported from IUCLID (substance DS / Endpoint study summaries):
  - Physical chemical properties and environmental fate properties
  - Toxicological / ecotoxicological properties
  - Environmental Hazard information:
    - PNEC value
    - standard justification why no PNEC available (from IUCLID 5 picklist)
  - Human Health Hazard information
    - DN(M)EL value
    - standard justification why no DN(M)EL available (from IUCLID 5 picklist)
- To ensure consistency in the data input, all data imported from IUCLID are not modifiable in Chesar.
- Identified uses can be exported from Chesar to section 3.5 in IUCLID



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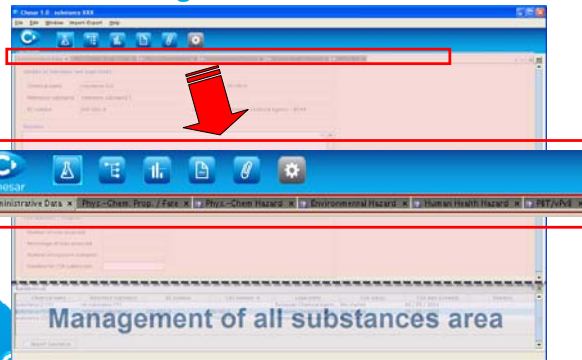
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## Box 1 - Manage substance tabs



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### ...in details :

- **Administrative Data** information related to the identity of the substance and the status of the CSA
- **Phys-Chem Prop. / Fate** contains the values for the physico-chemical and fate properties
- **Physical hazard** contains the values for the physico-chemical hazard properties, and enables the report of the C&L
- **Environmental Hazard** contains the PNECs (Predicted No Effects Concentrations) and the key ecotoxicological information, and enables the report of the C&L
- **Human Health Hazard** contains the DN(M)ELs (Derived No (or Minimum) Effect Levels), the key toxicological information, and enables the report of the C&L

PBT/vPvB enables the assessor justifying the (non) PBT/vPvB status of the substance



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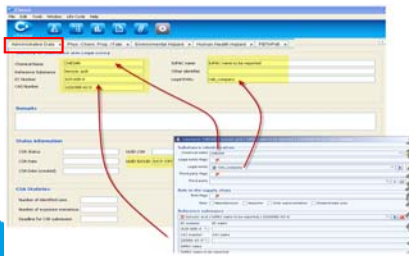
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### Administrative data – from IUCLID to Chesar

From IUCLID section 1.1



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### Phys-Chem mandatory to run the Chesar plugins

- (Molecular weight)
- Physical form of the substance
- Vapour pressure
- Water solubility
- Melting point
- Partition coefficient (Kow)
- Biodegradability in water (screening tests)

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Administrative Data	Value	Endpoint	Notes
Physical Form	liquid		
Molecular Weight	132.2 g/mol	EUH052.1	TBA workers
Melting Point	180 K w/ 101325 Pa	EUH051.1	
Boiling Point	444 K w/ 101325 Pa	EUH051.1	
Relative Density			
Vapour Pressure	2400 Pa w/ 298 K	EUH052.1	TBA workers
Partition Coefficient(Log Kow)	1.1 w/ 20 °C	EUH052.1	
Water Solubility	110 mg/L w/ 293 K	EUH052.1	
Solubility in standard fat			
Solubility in Organic Solvents			
Surface Tension			
Autoflammability/Self-ignition temperature			
Flammability			

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### Endpoint study summaries\* - from IUCLID to Chesar

- **Short description of key information** (*free text*): The content of this field will be transferred to the CSR (in the relevant section). A summary of the key information related to that endpoint should be reported here.
- **Key value for chemical safety assessment** (*numeric field or pick-list*): input for any calculation in Chesar. Consequently only a single value is to be reported in this field. When relevant the appropriate unit should also be filled-in.
- **Discussion** (*free text*): The content of this field will be transferred to the relevant section of the CSR as a summary of the assessment for the endpoint

\* Except PNECs / DN(M)EL endpoint summaries

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### An example....

**Endpoint summary: Vapour pressure**

Administrative Data: Short description of key information, Key value for chemical safety assessment, Discussion

Short description of key information: Vapour pressure < 0.01 Pa w/ 25°C. Information which will be reported in section 1 to 7 of the CSR as summary for the parameter!

Key value for chemical safety assessment: Vapour pressure: 0.01 Pa at the temperature of: 25 °C. Value selected for the assessment

Discussion: The substance has a very low vapour pressure... Discussion: reported in section 1 to 7 of the CSR

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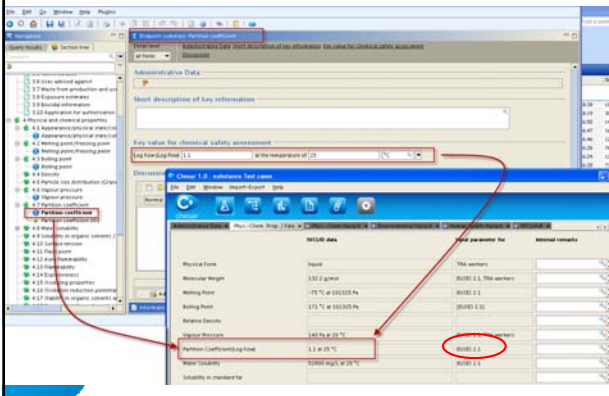
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## From IUCLID to Chesar (phys-chem prop/fate)




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## PNEC / DN(M)EL Endpoint study summary - from IUCLID to Chesar

- PNEC / DN(M)EL values, or
- Standard justification why no PNEC or DN(M)EL is available (IUC 5 picklist (e.g. "No dose response ..."), and
- Freetext




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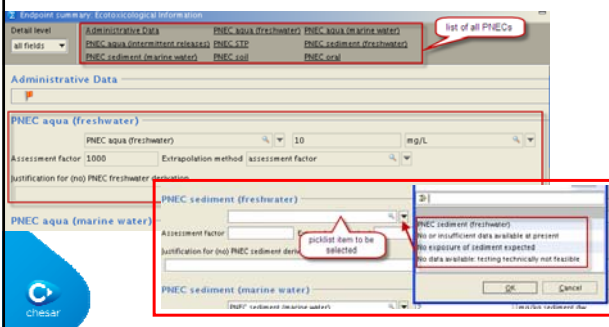
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## Environmental hazard: PNECs from IUC...

- Endpoint study summary 6: Ecotoxicological information




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## Scoping the exposure assessment

- The user manually indicates the **outcome of the hazard assessment** for:
  - Environment
  - Human health
- This information triggers in Chesar the adequate exposure assessment
  - Current approach (Chesar version 1.1.3):
    - Exposure assessment related to **chronic systemic** effects always required
    - Exposure assessment related to **acute** effects and **local effects** (on specific route) can be omitted based on the absence of classification
  - Future approach: Exposure assessment required, where
    - substance meets the criteria or being classified hazardous
    - other adverse effects have been observed up to limit dose/concentration of the relevant guideline study

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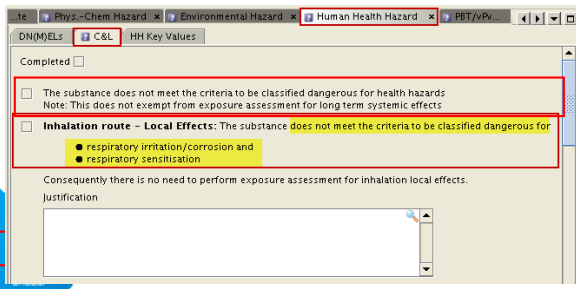
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## Scoping the assessment for HH

- Possibility to indicate whether the substance meets the criteria to be classified for **HH hazards** -> according to criteria described in 67/548/EEC and CLP




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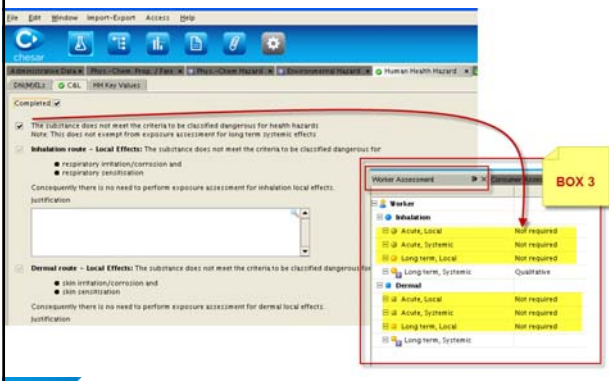
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## ...for example...




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## PBT/vPvB assessment

- Depending on the selection made by the assessor on the PBT/vPvB status (to be justified), Chesar triggers different assessment workflows:
  - If the first check box **Substance is regarded as PBT/vPvB** is ticked, Chesar triggers a 'PBT assessment'.



- If the second check box **Substance is not regarded as PBT/vPvB** is ticked, Chesar will trigger a 'standard assessment'.



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## To summarise (1)

- The IUCLID 5 substance information transferred to Chesar is:
  - Administrative data (from identity of the substance and LE section 1.1)
  - Molecular weight (from **reference substance** section 1.1)
  - Phys-Chemical properties (EPS 4) \*
  - Environmental data (PNECs) (EPS 6)
  - Human health data (DN(M)EL) (EPS 7)
- All data from IUCLID 5 are “read-only”

\* if the conditions of use do not correspond to the test then the properties of the substance under the actual conditions of use have to be determined



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## To summarise (2)

Before starting assessing the substance (Box 3), you should complete in Chesar (box 1) the following information:

- Hazard identification
  - phys-chem
  - ENV
  - HH
- Justification of the PBT/vPvB status



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### To summarise (3) – link between box 1 and 3

- Identified hazards (including classified hazards)
  - Determines the scope of exposure assessment in Box 3
  - Has to be activated by chesar user in Box 1
- Items picked from the DNEL/PNEC section in IUCLID
  - Determines the type of risk characterisation in Box 3
    - quantitative
    - qualitative
  - Determines the aim of the operational conditions and risk management measures in the exposure scenarios (Box 3)
    - Limit exposure to RCR < 1
    - Minimise exposure
  - Can be viewed from Box 1 but is automatically carried through to Box 3.



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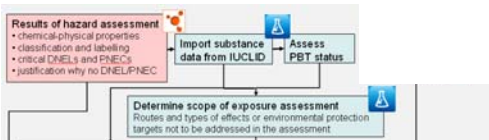
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### General Workflow



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Thank you for your attention  
Questions?



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