

# EUSES development plan and interlink with Chesar

Workshop on EUSES update needs

4 June 2018

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## Outline

- Introduction: High level ECHA's plans
- Chesar
- EUSES tool development: what are the critical choices?

# Introduction



## **EUSES tool technological state**

- EUSES was developed between 1994 (v1.0) and 2012 (version 2.1.2)
- Because of technological limitations, “EUSES engines” (equations) were re-implemented in different tools
  - excel for ECETOC TRA, EasyTRA
  - EUSES fate and exposure models have been recoded in java in Chesar
- The tool is not maintained. IT wise it is partly outdated.
- For biocides, there was an urgent need to implement the Emission scenario documents (ESDs):
  - ECHA has decided to take over the ownership of EUSES
  - The current tool is being extended (“quick fix” to be delivered in Q4 2018)



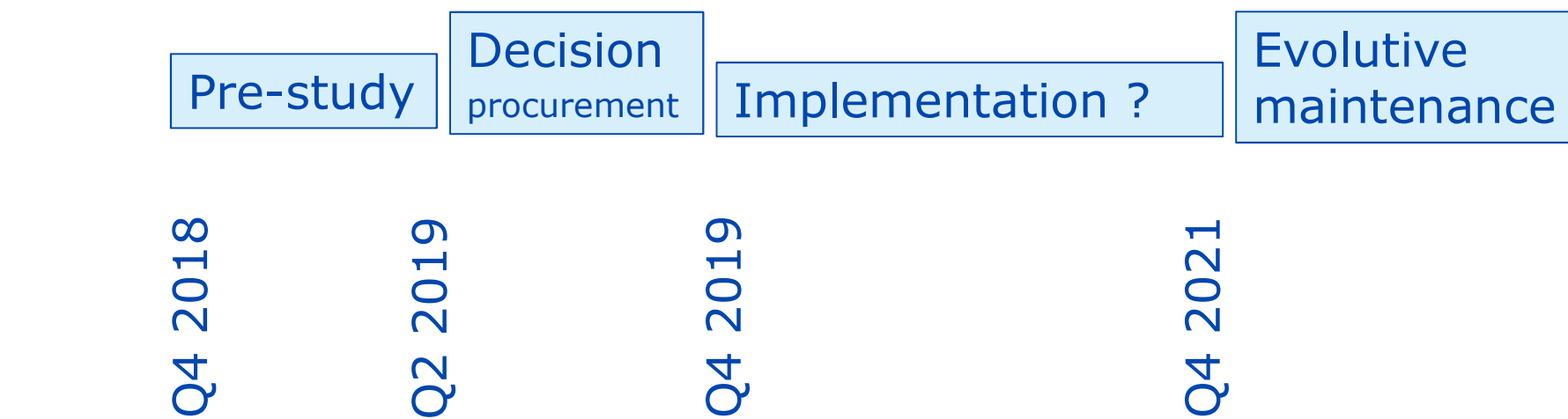
## **ECHA's plan regarding EUSES**

- ECHA's objective: maintain a tool for supporting harmonised and transparent environmental assessment -> efficient decision making in regulatory context
- Assessment of what should be done and related costs needed:
  - Collect information via this workshop
  - "Pre study"

## The “pre study”

- Analysis and design of new application taking into account the needs for changes
  - Understanding impact of changes proposed on IT code (design for the application)
    - Various (clearly defined) adaptations proposed
    - how to streamline the release module, in particular across REACH and biocide use
- How should the new EUSES be maintained?
  - Connection with other applications? (e.g. Chesar, IUCLID, other?)
- **Exact content of pre-study to be defined after the workshop**
- Involvement of (extended?) “organising committee” during pre-study.

# Timing



**Chesar**



## Chesar

- Chesar is a web application developed by ECHA **to support registrants under REACH** in consistently
  - carrying out their Chemical Safety Assessment
  - generating their Chemical Safety Report (CSR) as part of their registration
  - generating the Exposure Scenario for communicating conditions for safe use (annex to extended Safety Data Sheet)

## Organisation of Chesar: the Chesar “Boxes”



1. Substances
2. Uses
3. Exposure assessment
4. CSR
5. ES for extended SDS
6. Library
7. Users



chesar



Selected substance: ECHA substance

Selected CSA: default

Substance management

CSA management

Substance identity

Physico-chemical / fate properties

Fate in standard biological STP

Physico-chemical hazard

Hazard conclusion and scope of assessment

# Substance management ?

Import Chesar substance file

Import IUCLID substance dataset via web service

Search [Go to advanced search](#)

Search

Clear

Total 6

Previous

1

Next

Chemical name	Reference substance	EC number	CAS number
Complex case example – Substance which transforms	Parent substance		
ECHA substance	ECHA Substance		11111-11-1



Selected substance: ECHA substance Selected CSA: default

Substance management

CSA management

Substance identity

Physico-chemical / fate properties

Fate in standard biological STP

Physico-chemical hazard

Hazard conclusion and scope of assessment

General

Biodegradation

Bioaccumulation

Abiotic degradation

Adsorption

Property name

Value

Physical form

liquid

Molecular weight (upper limit)

Molecular weight (lower limit)

300

Molecular weight (for assessment)

300

Melting point at 101 325 Pa

219 K

Boiling point at 101 325 Pa

519 K





chesar

Selected substance: ECHA substance Selected CSA: default



Substance management

CSA management

Substance identity

Physico-chemical / fate properties

Fate in standard biological STP

Physico-chemical hazard

Hazard conclusion and scope of assessment

## Release percentages of modelled biolog

### ECHA substance

- Default EUSES settings
- Specific settings

Apply

Release (%) directed to water	77.84
Release (%) directed to air	13.64
Release (%) directed to sludge	8.514
Release (%) degraded	0
Total	100 %

Save



chesar

Selected substance: **ECHA substance** Selected CSA: **default**



Substance management

CSA management

Substance identity

Physico-chemical / fate properties

Fate in standard biological STP

Physico-chemical hazard

Hazard conclusion and scope of assessment

## Release percentages of modelled biolo

**ECHA substance**

Default EUSES settings  
 Specific settings

Apply	
Release (%) directed to water	<input type="text"/>
Release (%) directed to air	<input type="text"/>
Release (%) directed to sludge	<input type="text" value="8.514"/>
Release (%) degraded	<input type="text" value="0"/>
Total	%

Save

Substance management

CSA management

Substance identity

Physico-chemical / fate  
properties

Fate in standard biological  
STP

Physico-chemical hazard

Hazard conclusion and  
scope of assessment

**Environment**

Workers

Consumers

Man via environment



## PBT assessment

ECHA substance

The substance is not PBT / vPvB

## Hazard for Aquatic organisms

### Compartment

### Hazard conclusion


Freshwater

PNEC aqua (freshwater) **0.01 mg/L** 

Sediment (freshwater)

PNEC sediment (freshwater) **0.837 mg/kg sedime**  
Extrapolation method: **equilibrium partitioning m**

Marine water

PNEC aqua (marine water) **1.03E-3 mg/L** 

Sediment (marine water)

PNEC sediment (marine water) **0.084 mg/kg sedin**  
Extrapolation method: **equilibrium partitioning m**

Sewage treatment plant (STP)


PNEC STP **1.49 mg/L** 

## Hazard for Air

### Compartment

### Hazard conclusion

Air

No hazard identified 

chesar  
Selected substance: ECHA substance Selected CSA: default

Import life cycle tree Export life cycle tree

- Manuf.Imp (320 t) : Manufacture / Im...
- Manuf. (320 t) : Manufacture
- Formul. (320 t) : Formulation o...**
  - ERC 2: Formulation of mixt...**
  - PROC 8b: Receiving and c...
  - PROC 3: Mixing or blending...
  - PROC 5: Mixing or blending...
  - PROC 8a: Transfer of subst...
  - PROC 8b: Transfer of subst...
  - PROC 9: Transfer of substa...
  - PROC 28: Equipment clean...
- Market (200 t) : Coatings and Inks

## Edit use: *Formulation of liquid m*

⚠ Show additional fields relevant for use description in IUCLID

Name:

Formulation of liquid mixtures

Further description of use:

**B** *I* U ☰ ☰☰☰ ↺

Formulation refers to the mixing of raw materials, coatings, inks, lubricants, and filling containers.

Formulation steps that require worker intervention, such as manual batch processes; non-automated transfer and cleaning operations are also included.

# Box 3: release/exposure estimation

The screenshot displays the chesar software interface. At the top, a navigation bar includes icons for home, flask, menu, a highlighted bar chart icon, document, paperclip, settings, users, and help. Below the navigation bar, the text "Selected substance: ECHA substance" and "Selected CSA: default" is visible. Two buttons are present: "Add default exposure datasets" and "Bulk edit mode".

The main content area features a workflow diagram with three steps: "Release and exposure" (highlighted with a red box), "Risk characterisation", and "exposure estimates information" (also highlighted with a red box). Below this, the "Conditions of use" section is highlighted with a red box and contains a sub-section "Releases" (also highlighted with a red box). The "Exposure estimates" section is also highlighted with a red box.

On the left side, a sidebar lists various processes with status indicators (checkmarks and wrench icons):

- Environmental assessment for aggre...
- Manuf. (320 t) : Manufacture
- Formul. (320 t) : Formulation of liq...
- ERC 2: Formulation of mixt...**
- PROC 8b: Receiving and cha...
- PROC 3: Mixing or blending i...
- PROC 5: Mixing or blending i...
- PROC 8a: Transfer of substa...
- PROC 8b: Transfer of substa...
- PROC 9: Transfer of substanc...
- PROC 28: Equipment cleanin...
- Market (200 t) : Coatings and Inks

At the bottom of the interface, a large blue text block reads: "Daily intake via food item estimated by EUSES 2.1.2".



## Conditions of use

Conditions based on

E-W-1 : Product (article) characteristics

E-W-2 : Amount used, frequency and duration of use (or from service life)

Daily use amount at site  $\leq$   tonnes/day 

Annual use amount at site  $\leq$   tonnes/year 

E-W-3 : Technical and organisational conditions and measures

E-W-4 : Conditions and measures related to biological sewage treatment plant

Biological STP  Wat. effect.. :  % 

Discharge rate of STP  $\geq$   m<sup>3</sup>/day 

Application of the STP sludge on agricultural soil  

# Releases ?

## Releases before modelled biological STP

Release route	Estimation method	Release factor		Release rate		
		before on-site RMM	after on-site RMM	local	regional	
Water	ERC based	2 %	2 %	64 kg/day	17.53 kg/day	
Air	ERC based	2.5 %	2.5 %	80 kg/day	21.91 kg/day	
Soil	ERC based		0.01 %		0.088 kg/day	

Release factor to external waste  %

## Releases from the local modelled biological STP

Release route	Release rate
Water	49.82 kg/day
Air	8.731 kg/day
Agricultural soil via application of sludge	5.449 kg/day

## Exposure estimates ?

Add new exposure dataset ▼

Delete dataset ▼

Compartment	Method <span style="color: grey;">▼</span>	Status <span style="color: grey;">▼</span>	CLocal	PEC/Exposure	RCR
<b>Environmental exposure estimates <span style="color: grey;">▼</span></b>					
Fresh water <span style="color: grey;">▼</span>	EUSES 2.1.2	Main <span style="color: grey;">▼</span>	2.488 mg/L	2.488 mg/L	241.5 <span style="color: red;">⚠</span>
Sediment (freshwater) <span style="color: grey;">▼</span>	EUSES 2.1.2	Main <span style="color: grey;">▼</span>		202.0 mg/kg dw	241.3 <span style="color: red;">⚠</span>
Marine water <span style="color: grey;">▼</span>	EUSES 2.1.2	Main <span style="color: grey;">▼</span>	0.249 mg/L	0.249 mg/L	241.5 <span style="color: red;">⚠</span>
Sediment (marine water) <span style="color: grey;">▼</span>	EUSES 2.1.2	Main <span style="color: grey;">▼</span>		20.20 mg/kg dw	241.3 <span style="color: red;">⚠</span>
Sewage Treatment Plant <span style="color: grey;">▼</span>	EUSES 2.1.2	Main <span style="color: grey;">▼</span>		24.91 mg/L	16.71 <span style="color: red;">⚠</span>
Agricultural soil <span style="color: grey;">▼</span>	EUSES 2.1.2	Main <span style="color: grey;">▼</span>	9.807 mg/kg dw	9.807 mg/kg dw	60.91 <span style="color: red;">⚠</span>
<b>Man via environment exposure estimates <span style="color: grey;">▼</span></b>					
Man via environment - Inhalation <span style="color: grey;">▼</span>	EUSES 2.1.2	Main <span style="color: grey;">▼</span>		6.09E-3 mg/m <sup>3</sup>	1E-3 <span style="color: green;">✔</span>
Man via environment - Oral <span style="color: grey;">▼</span>	EUSES 2.1.2	Main <span style="color: grey;">▼</span>		5.267 mg/kg bw/day	1.505 <span style="color: red;">⚠</span>
Man via environment - Combined <span style="color: grey;">▼</span>					1.506 <span style="color: red;">⚠</span>





chesar



Selected substance: ECHA substance Selected CSA: default

Generate CSR ▾

Export uses to IUCLID

### 9.1.1.2. Releases

The local releases to the environment are reported in the following table. Note that the releases reported do not account for the removal in the modelled biological STP.

Table 9.7. Local releases to the environment

Releases	Release estimation method	Explanations
Water	Estimated release factor (Manufacturing site specific)	<b>Release factor before on site RMM: 0%</b> <b>Release factor after on site RMM: 0%</b> <b>Local release rate: 0 kg/day</b> <b>Explanation:</b> No water used in the process or for cleaning equipment/maintenance operation.
Air	ERC	<b>Release factor before on site RMM: 5%</b> <b>Release factor after on site RMM: 0.05%</b> <b>Local release rate: 8 kg/day</b>
Non agricultural soil	Estimated release factor (Manufacturing site specific)	<b>Release factor after on site RMM: 0%</b> <b>Explanation:</b> Closed system. No release to soil.

### 9.1.1.3. Exposure and risks for the environment and man via the environment

The exposure concentrations and risk characterisation ratios (RCR) are reported in the following table. The exposure estimates have been obtained with EUSES 2.1.2 unless stated otherwise.

Table 9.8. Exposure concentrations and risks for the environment and man via the environment

Protection targets	Exposure concentration	Risk quantification
Fresh water	Local PEC: 3.93E-5 mg/L	RCR < 0.01
Sediment (freshwater)	Local PEC: 3.19E-3 mg/kg dw	RCR < 0.01
Marine water	Local PEC: 3.52E-6 mg/L	RCR < 0.01
Sediment (marine water)	Local PEC: 2.85E-4 mg/kg dw	RCR < 0.01

## Chesar: assessment of “complex cases”

- In some situations **several sets of information** on substance properties may play a role for conducting the exposure and risk assessment of a registered substance, e.g.:
  - Different forms/compositions with different hazard profile
  - Substance “transforming” into another substance
  - Substance composed of many constituents (including UVCB)
- Creation of Assessment Entities (AE) in IUCLID
- Assessment for (groups of) assessment entities in Chesar
- More information:
  - Chapter D2 of Guidance part D:  
[https://echa.europa.eu/documents/10162/13632/information\\_requirements\\_part\\_d\\_en.pdf](https://echa.europa.eu/documents/10162/13632/information_requirements_part_d_en.pdf)
  - Manual “How to prepare registration and PPORD dossiers”:  
<https://echa.europa.eu/manuals>
  - Chesar 3 manual, chapter 9: <https://chesar.echa.europa.eu/support/manuals-tutorials>
  - Helptext in Chesar (visible when AE have been imported)

General

Biodegradation






















Bioaccumulation

Abiotic degradation

Adsorption coefficients




Property name	AE3 abietane block	AE1 C18 fatty acid	Rosin	AE4Pimarane block
Physical form	liquid	liquid	liquid	liquid
Molecular weight (upper limit)			414.7	
Molecular weight (lower limit)	300.4	280.4	258.3	100
Molecular weight (for assessment)	303.1	281.4	414.7	133.3
Melting point at 101 325 Pa	93.4 °C	93.4 °C		93.4 °C
Boiling point at 101 325 Pa	400 °C	390 °C		390 °C
Relative density at 20 °C	1.03E3	1.03E3		1.03E3
Vapour pressure	1.3E-3 Pa at 25 °C	4E-3 Pa at 25 °C	1E-3 Pa at 25 °C	1.8E-3 Pa at 25 °C
Partition coefficient (Log Kow)	4.1 at 25 °C	5.4 at 25 °C		4.2 at 25 °C
Water solubility	84 mg/L at 20 °C	1.1 mg/L at 20 °C		7.7 mg/L at 20 °C

Compartment	Assessment entity	Method 	CLocal	PEC/Exposure	RCR	RCR across AE
<b>Environmental exposure estimates </b>						
Fresh water 	AE1 C18 fatty acid	<a href="#">EUSES 2.1.2</a>	3.55E-4 mg/L	3.62E-4 mg/L	0.157 	1.272 
	AE3 abietane block	<a href="#">EUSES 2.1.2</a>	7.73E-3 mg/L	7.9E-3 mg/L	0.444 	
	AE4Pimarane block	<a href="#">EUSES 2.1.2</a>	0.011 mg/L	0.011 mg/L	0.67 	
Sediment (freshwater) 	AE1 C18 fatty acid	<a href="#">EUSES 2.1.2</a>		0.245 mg/kg dw	0.885 	0.971 
	AE3 abietane block	<a href="#">EUSES 2.1.2</a>		1.149 mg/kg dw	0.032 	
	AE4Pimarane block	<a href="#">EUSES 2.1.2</a>		1.809 mg/kg dw	0.055 	
Marine water 	AE1 C18 fatty acid	<a href="#">EUSES 2.1.2</a>	3.55E-5 mg/L	3.62E-5 mg/L	0.157 	1.271 
	AE3 abietane block	<a href="#">EUSES 2.1.2</a>	7.73E-4 mg/L	7.89E-4 mg/L	0.443 	
	AE4Pimarane block	<a href="#">EUSES 2.1.2</a>	1.08E-3 mg/L	1.11E-3 mg/L	0.67 	
Sediment (marine water)	AE1 C18 fatty acid	<a href="#">EUSES 2.1.2</a>		0.024 mg/kg dw	0.883 	0.97 
	AE3 abietane block	<a href="#">EUSES 2.1.2</a>		0.115 mg/kg dw	0.032 	
	AE4Pimarane block	<a href="#">EUSES 2.1.2</a>		0.181 mg/kg dw	0.055 	

# Chesar provides opportunities for

- Consistency
  - Within the CSA: substance properties, uses reported in IUCLID and the chemical safety report
  - Information for the authorities (CSR) and for the supply chain (exposure scenario for communication)
- Standardisation (efficiency gains for all actors)
  - Systematic workflow
  - Import/export/printed format of Use maps, Chemical safety report, Exposure scenarios for communication (Standard phrases: ESCom)
- Efficiency in single assessment
  - Integrated exposure estimation tools
  - Re-use of information across substances
  - Automated generation of documents
  - Facilitated updates

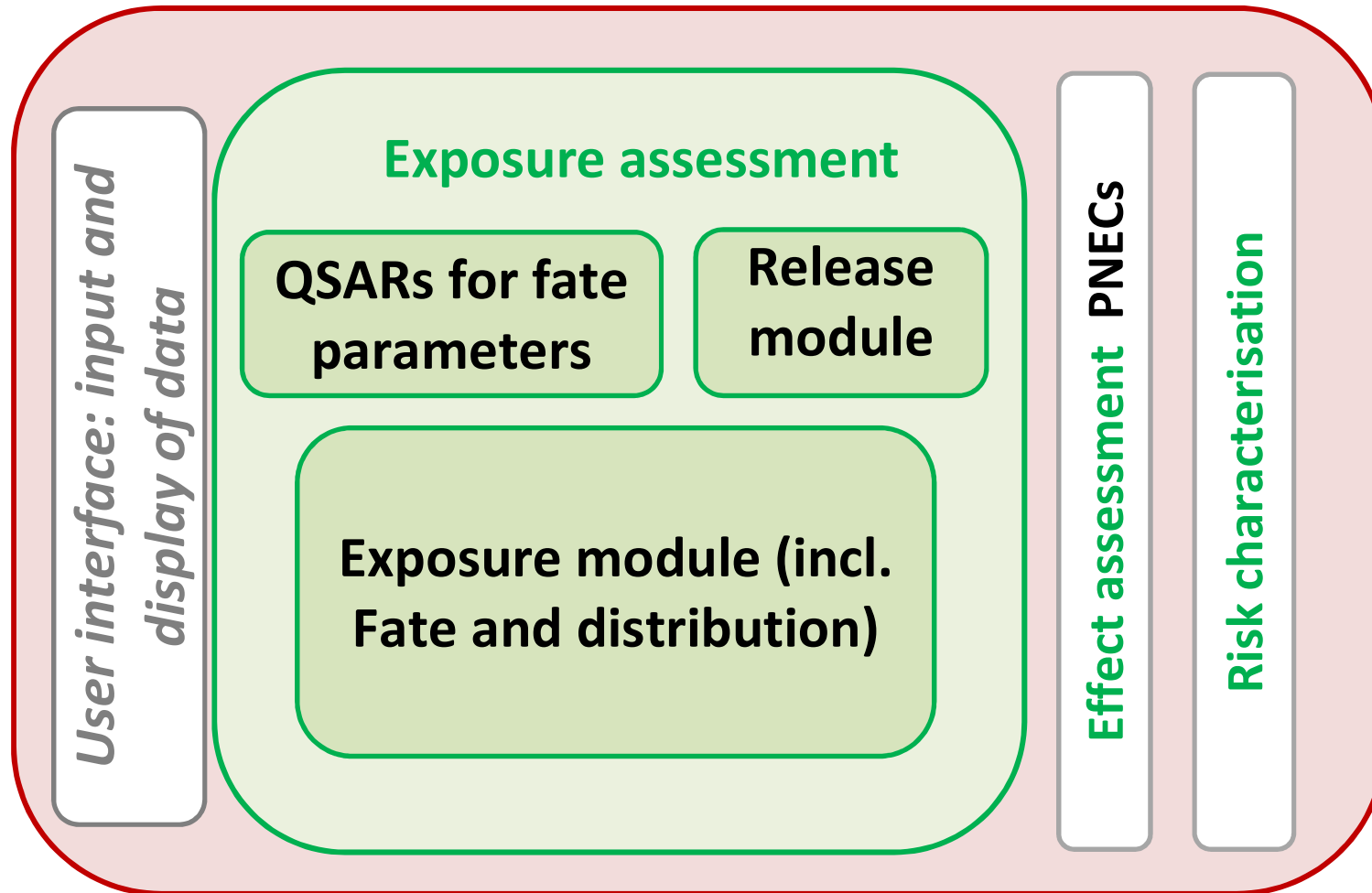
## More information

- Chesar user manual  
<https://chesar.echa.europa.eu/support/manuals-tutorials>
- Helptext within the application : 
- Webinars have been recorded

**EUSES tool development: what are the critical choices?**

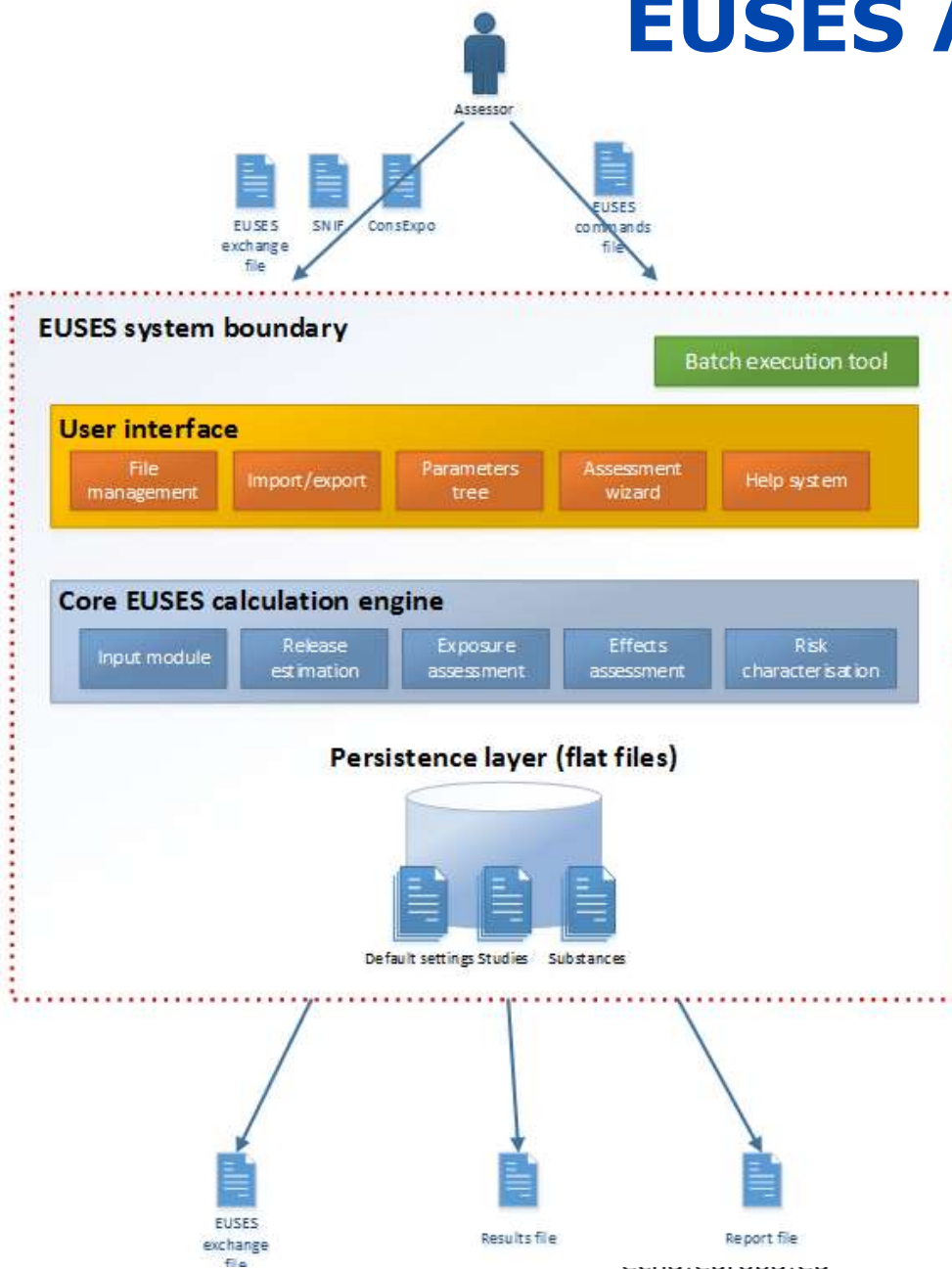


# EUSES high level structure



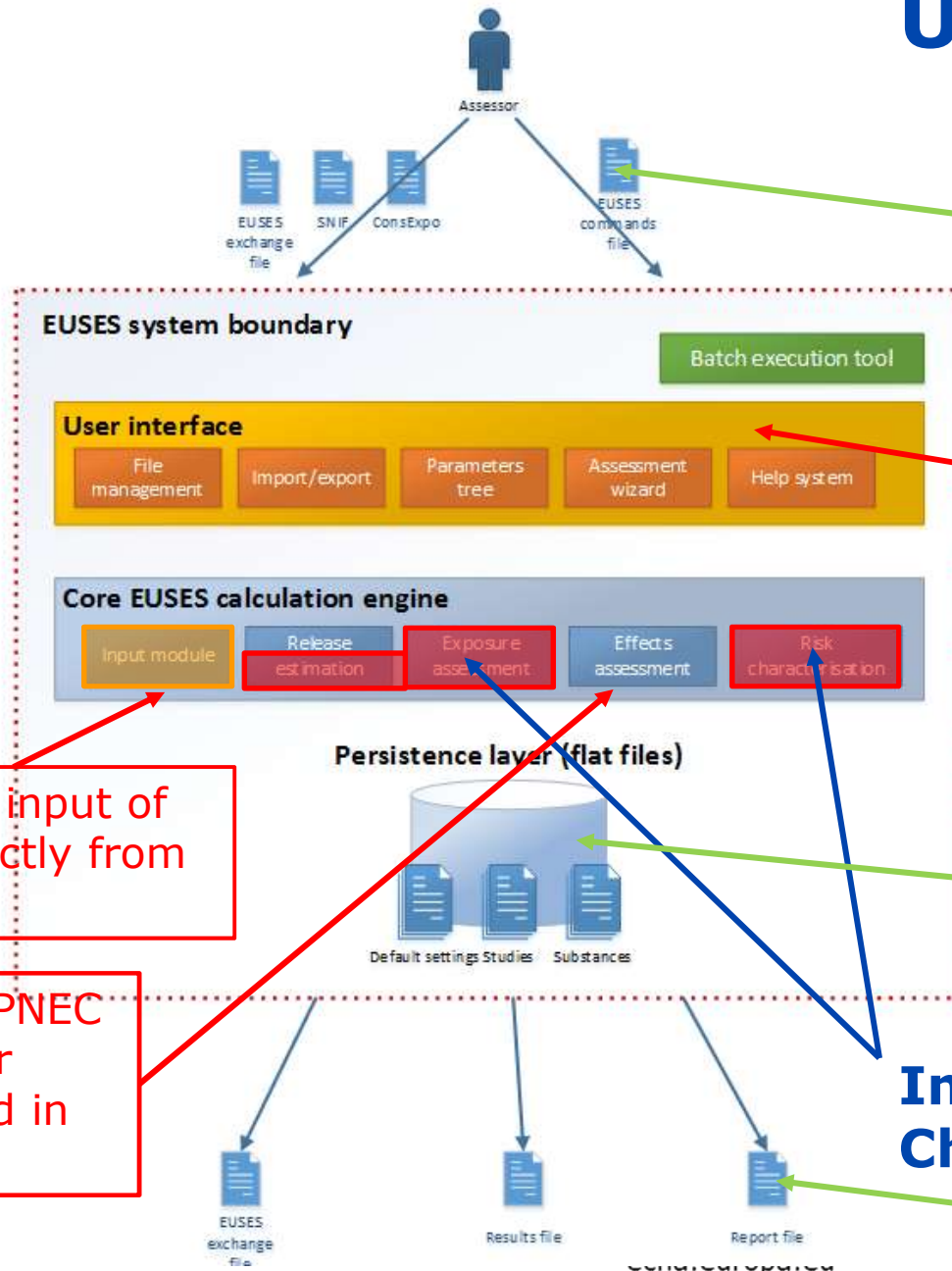


# EUSES Architecture



**EASE** also OUT OF SCOPE

# Usage of EUSES



Is there a need to import data?

Is there a need for an own user interface? (or can be integrated e.g. in Chesar)

Enabling input of data directly from IUCLID?

Reusing PNEC calculator imbedded in IUCLID?

Is there a need to save the data in DB?

**Implemented in Chesar**

Is there a need to export data?

## ECHA baseline for future developments

- Starting from the extraction of EUSES calculation engine re-implemented inside Chesar, what shall ECHA do for v3.0?
  - Modify/extend the calculation engine (content modifications) ?
  - Modify the usability (e.g. user interface, reporting functionalities)
  - Maintain a standalone version?
  - Facilitate to re-use of the calculation engine in other tool?

## Future evolutive maintenance

How to anticipate release sequence (expected frequency of releases):

- Changes to calculation engine
  - to take place between v2.0.0 and 3.0.0
  - nothing foreseen after (should be in v4.0) as past calculation might be different
- Extensions to calculations v3.X.y (e.g. new release scenario, new model, extension of applicability domain to other substances)
- Technical changes v3.x.Y (e.g. new functionalities, bug correction)

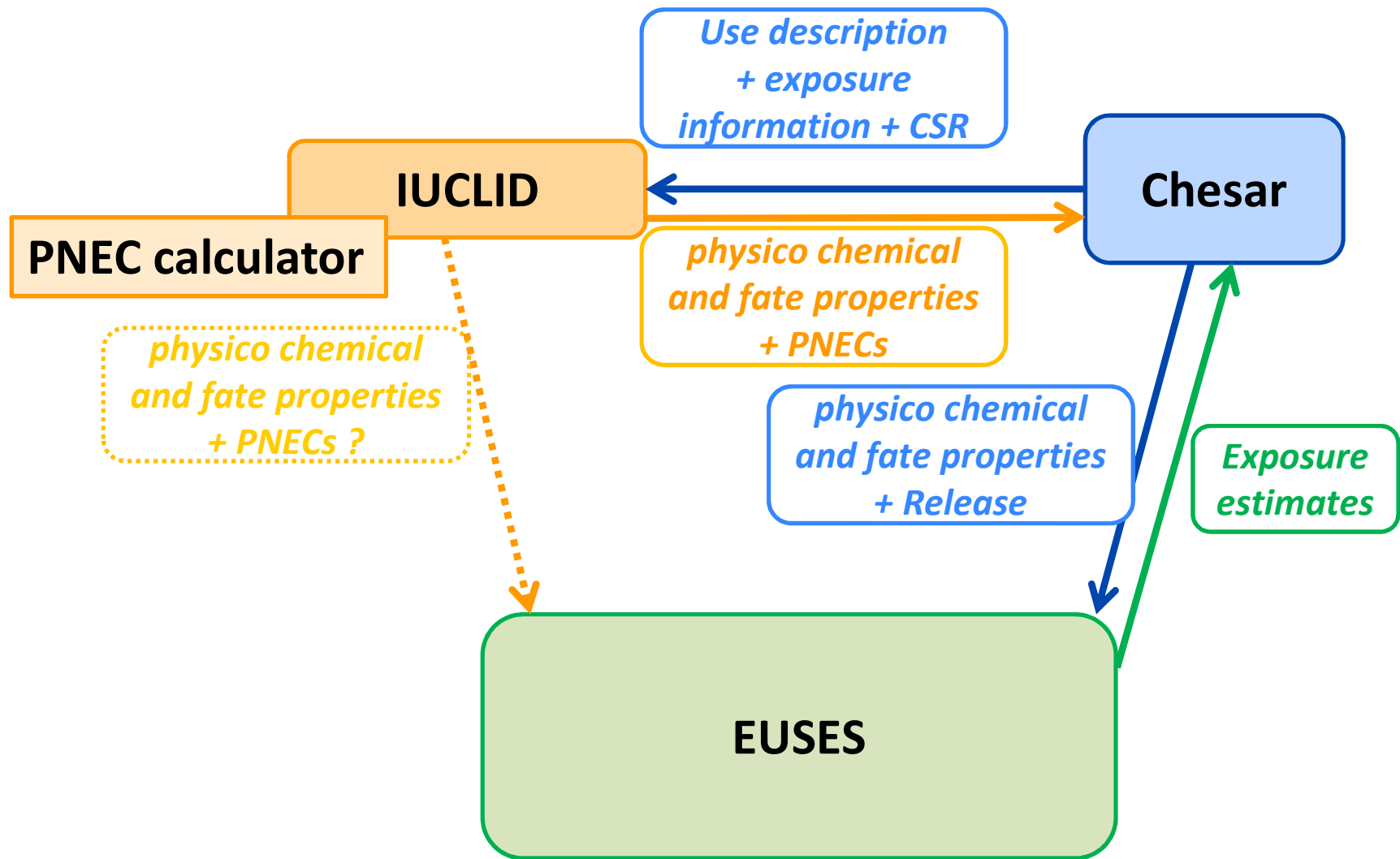
## Candidate IT options for standalone version

	<b>Local version</b>	<b>On-line version</b>
Internet connection	Not needed	Needed
Installation	By user	Not needed
Updates	Require new installation	Carried by host. Not "visible" by user
Data	Stored locally: accessible only from own computer	At host (dedicated access): accessed from any computer
Maintenance	Via helpdesk and releases	Dedicated support and fast correction

## User access to EUSES

- Need for a standalone version of EUSES (own user interface)?
- Would it be acceptable if access of EUSES done via Chesar (to be extended to fit other needs)?

	<b>Current standalone EUSES</b>	<b>Current Chesar</b>
Workflow	Data screen by data screen	More high level workflow
Editability of parameters	All parameters editable, clear differentiation between parameters <b>default</b> or <b>output or set</b> by the user	Only selected parameters editable Possibility to report explanations/choices
Tiered approach	All parameters have same "status"	<ul style="list-style-type: none"> <li>• Release (ERC/SPERC/measured)</li> <li>• STP characterisation (local/generic)</li> </ul>
Reporting	basic	Automated generation of report (CSR, could be CAR)



## Other applications access to EUSES

- Is there a need for access to EUSES calculation engine for other applications (beyond Chesar)?

	re-usable API libraries	Local web-services	On-line web-services
Internet access	No internet need	No internet need	Internet need
EUSES updates (minor changes)	Re-packaging needed	Re-installation of EUSES	No change needed



## World Café session tomorrow

- Interactive discussion on presentation topics
  - Additional explanations
  - Clarifications
- Aiming at defining IT priorities for ECHA
  - Analysing expectations
  - Presenting alternatives

# Thank you!

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