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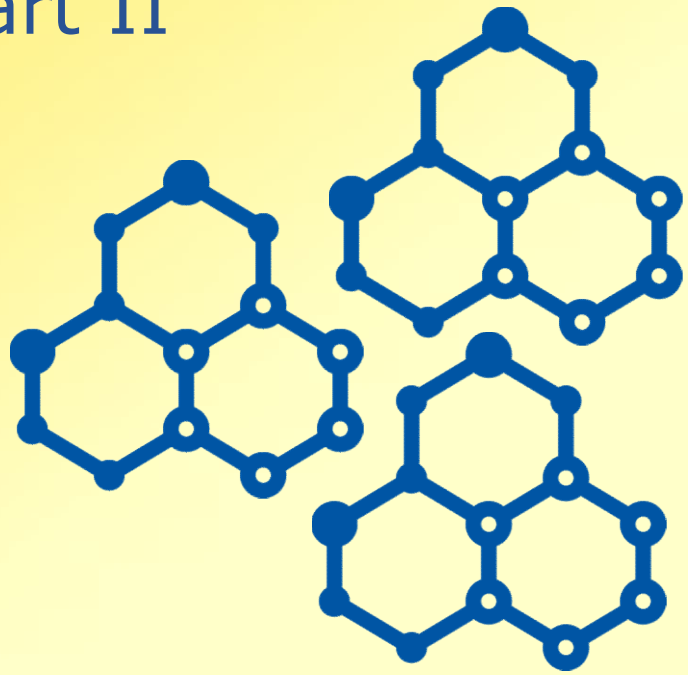
European Union System for the Evaluation of Substances

Current limitations and update needs identified by workshop organising committee - Part II

EUSES Update workshop
4 June 2018



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Sediment/water

- **14. Marine versus freshwater sediment**
- **15. PECregional, sediment**
- **16. Nested local scale multimedia model**

Frederik Verdonck

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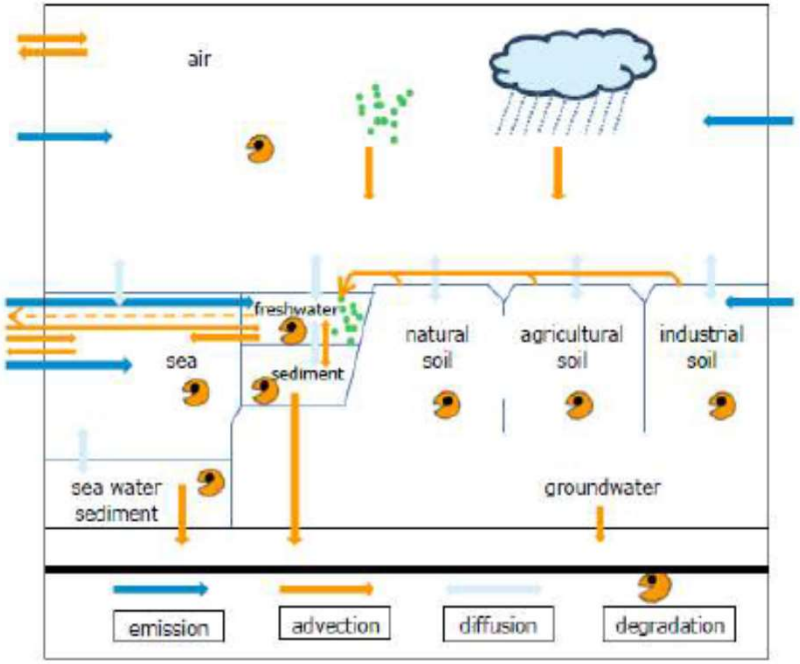
Current situation

Regional assessment



- **Kp** is same for freshwater and marine sediment PEC calculation
- Fully interlinked compartments

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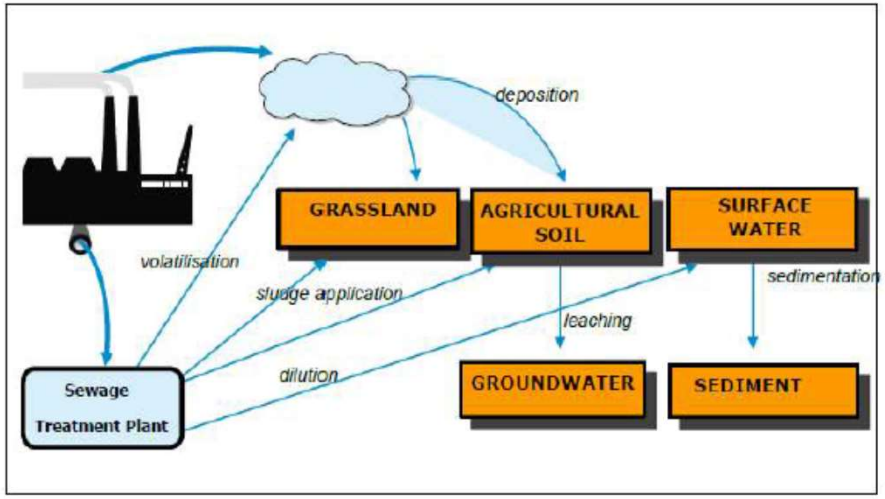
Current situation

Local assessment



- **Kp** is same for freshwater and marine sediment PEC calculation
- The regional PECsediment is not used in local PECsediment calculation

$$PEClocal_{sed} = \frac{K_{susp-wate}}{RHO_{susp}} \cdot \left(Clocal_{(sea)water} + PECregional_{water}\right) \cdot 1000$$

- Model concept: "separate" one compartment models

Change proposed

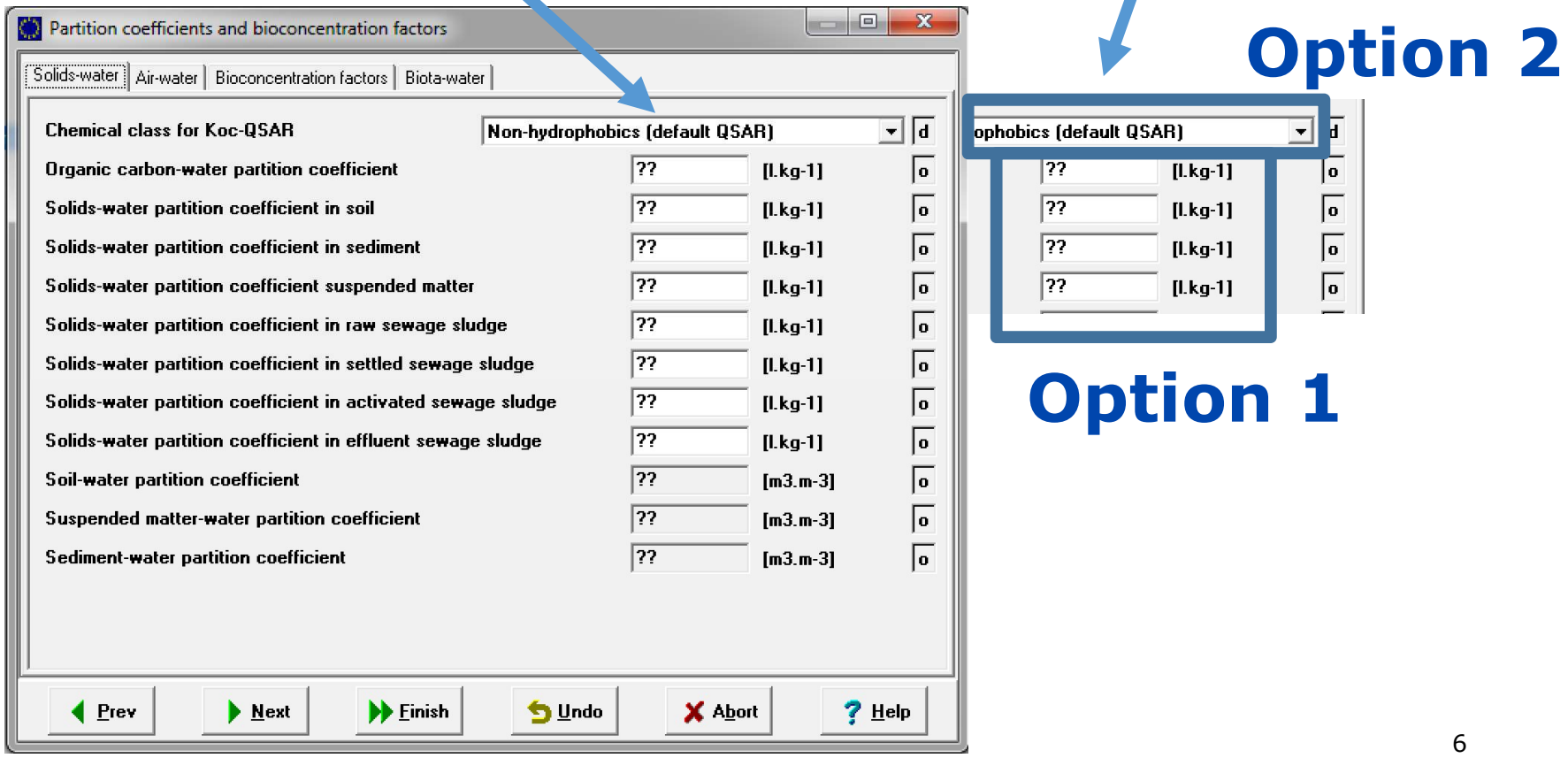
Different Kp(susp) and Kp(sed) for seawater and freshwater

- Option 1: Include separate Kp for marine compartment (default: Kp marine = Kp freshw)

- Option 2: Improve the environmental characteristics of the marine water and sediment compartments in order to improve default calculation of the Kp(susp) and Kp(sed) for marine environment

Change proposed

Different Kp(susp) and Kp(sed) for seawater and freshwater



Change proposed

Nested local scale multimedia model

- **Option 1**: Improve local scale model by taking improved items from option 2:
  - Two compartment water/sediment model
  - Consideration of additional fate processes
  - Improved air deposition
  - Nesting local scale model

- **Option 2**: Complete nested local scale multimedia model

Nested local scale model

Consideration of additional fate processes

Change proposed

Fate process	Flowing water body			'Static' water body	
	EUSES	PT 8 ESD		PT 8 ESD	
	Local scale	Tier 1	Tier 2	Tier 1	Tier 2
Adsorption/desorption suspended matter	**X**		**X**		**X**
Sedimentation and resuspension					To be considered as higher tier
Degradation in water (removal from water column)	To be considered as higher tier?	**X**	**X**	**X**	**X**
Adsorption/desorption sediment	**(X)**	**(X)**	**(X)**	**(X)**	**X**
Degradation in sediment					
Sediment burial	To be considered as higher tier?		To be considered as higher tier?		To be considered as higher tier
Irreversible binding to minerals = ageing	To be considered as higher tier?		To be considered as higher tier?		To be considered as higher tier

Why to propose change

Proposed update	Benefit
Different Kp for freshwater/marine	Allows to differentiate between seawater and freshwater where partitioning behaviour is different
PECregional sediment in PEClocal	Improved local PEC sediment (in case of measured regional PEC sediment)
Nested local multimedia scale model	Improved local PEC calculation

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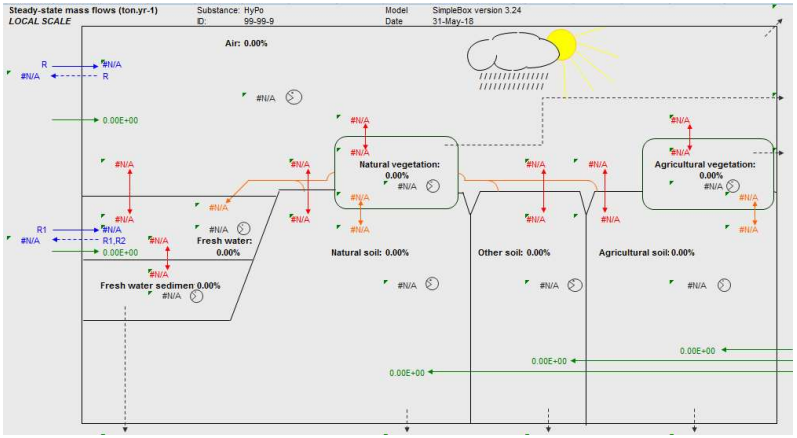
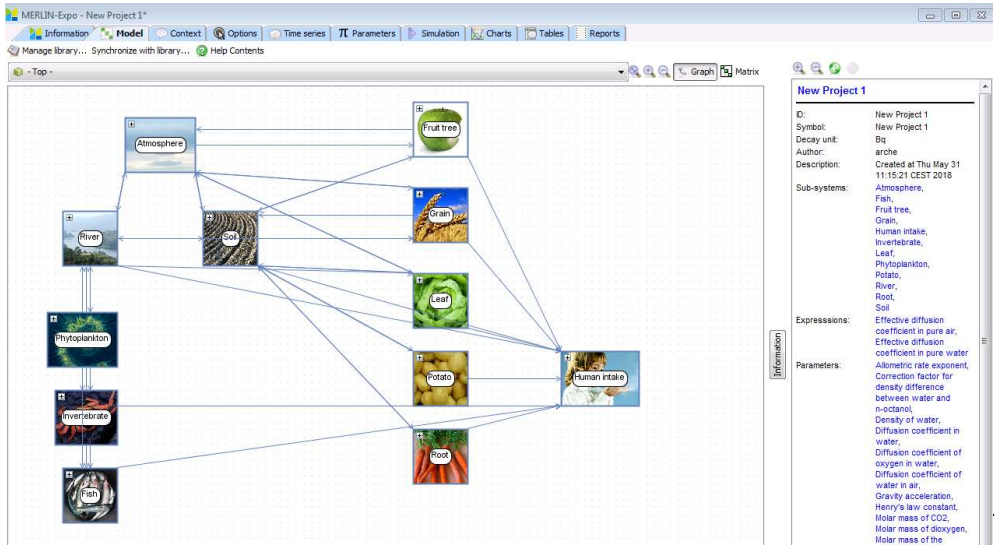
Support for implementation

- ESD PT8
- spreadsheet version 3.0 of Simplebox
- MERLIN EXPO





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Conclusions

Proposed update	Proposed priority
Different Kp for freshwater/marine Option 1: user-input Option 2: QSAR calc	 Ready / important Not ready / low importance
PECregional sediment in PEClocal	Ready / important
Nested local scale Option 1: light Option 2: full	 Not ready / important Not ready / low importance

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Man via the environment

- **17. Man indirectly exposed via the environment**
- **18. Man via the environment: alternative model for crop exposure pathway**

Frederik Verdonck &
Joost Bakker

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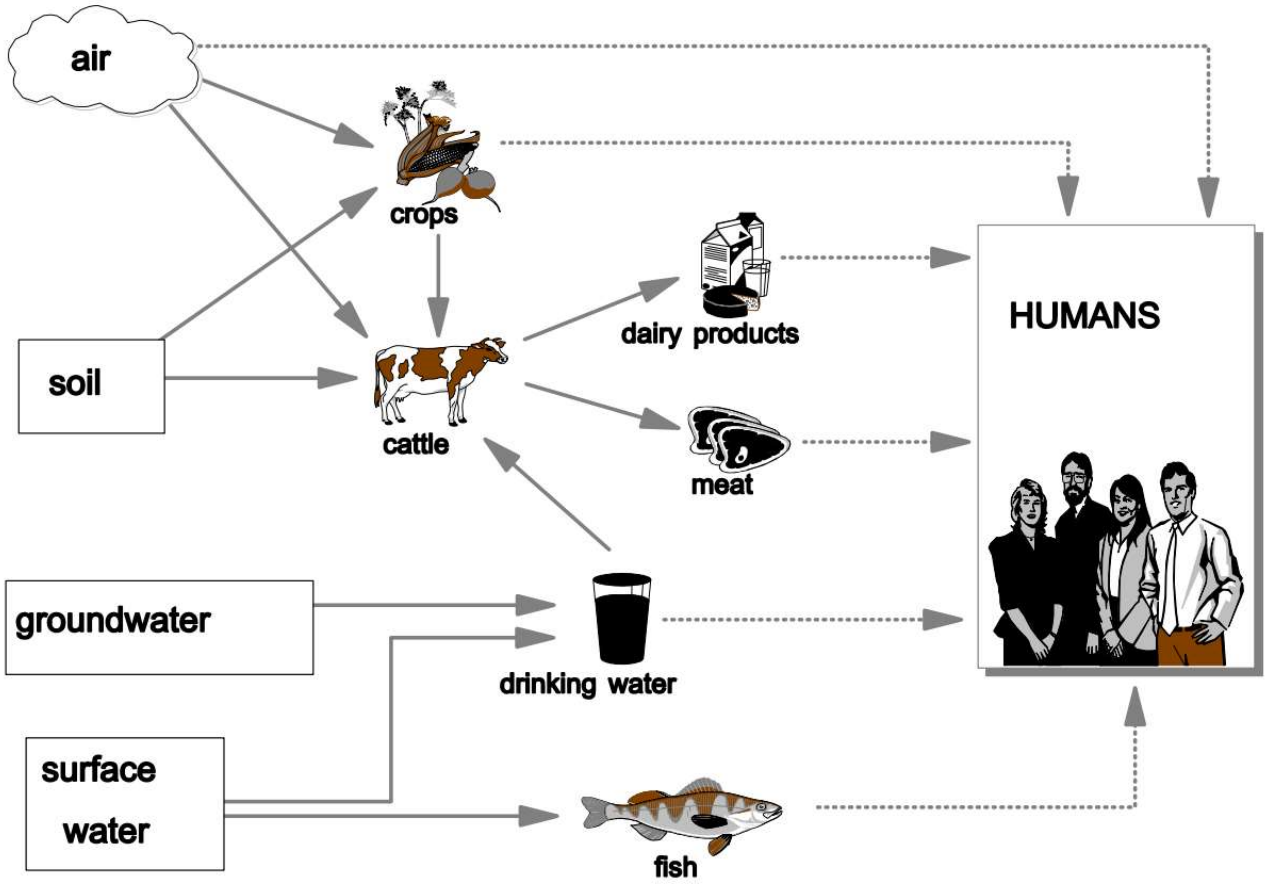
Man (indirectly exposed) via the environment scenario



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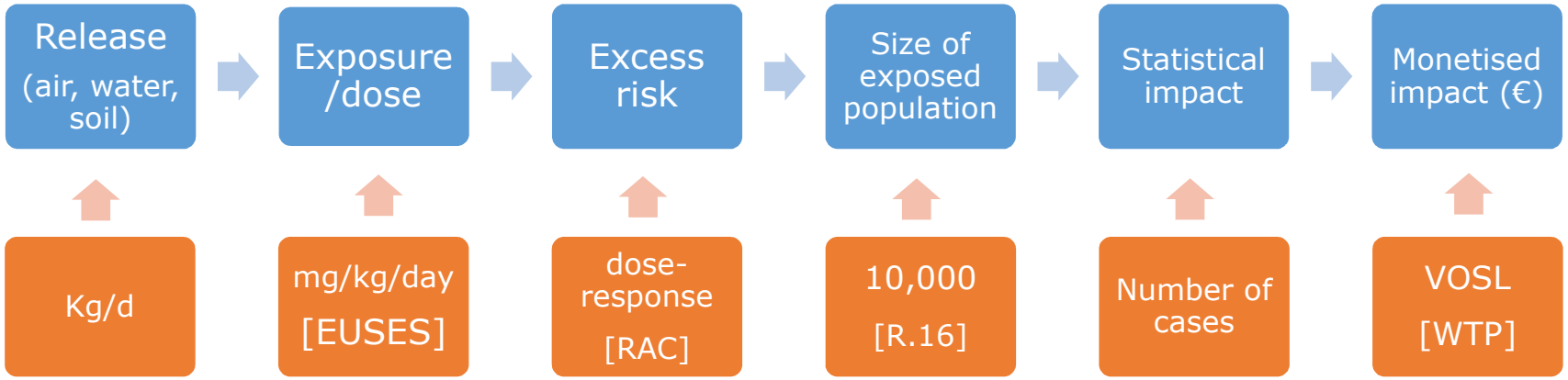
Importance of MvE scenario

- Standard default scenario REACH / BPR
- Usually environment is driving risk assessment
- More important under REACH Authorization:

Worker	**0.006**	2300	13
MvE local	8.3×10^{-5}	15,900,000	**1314**



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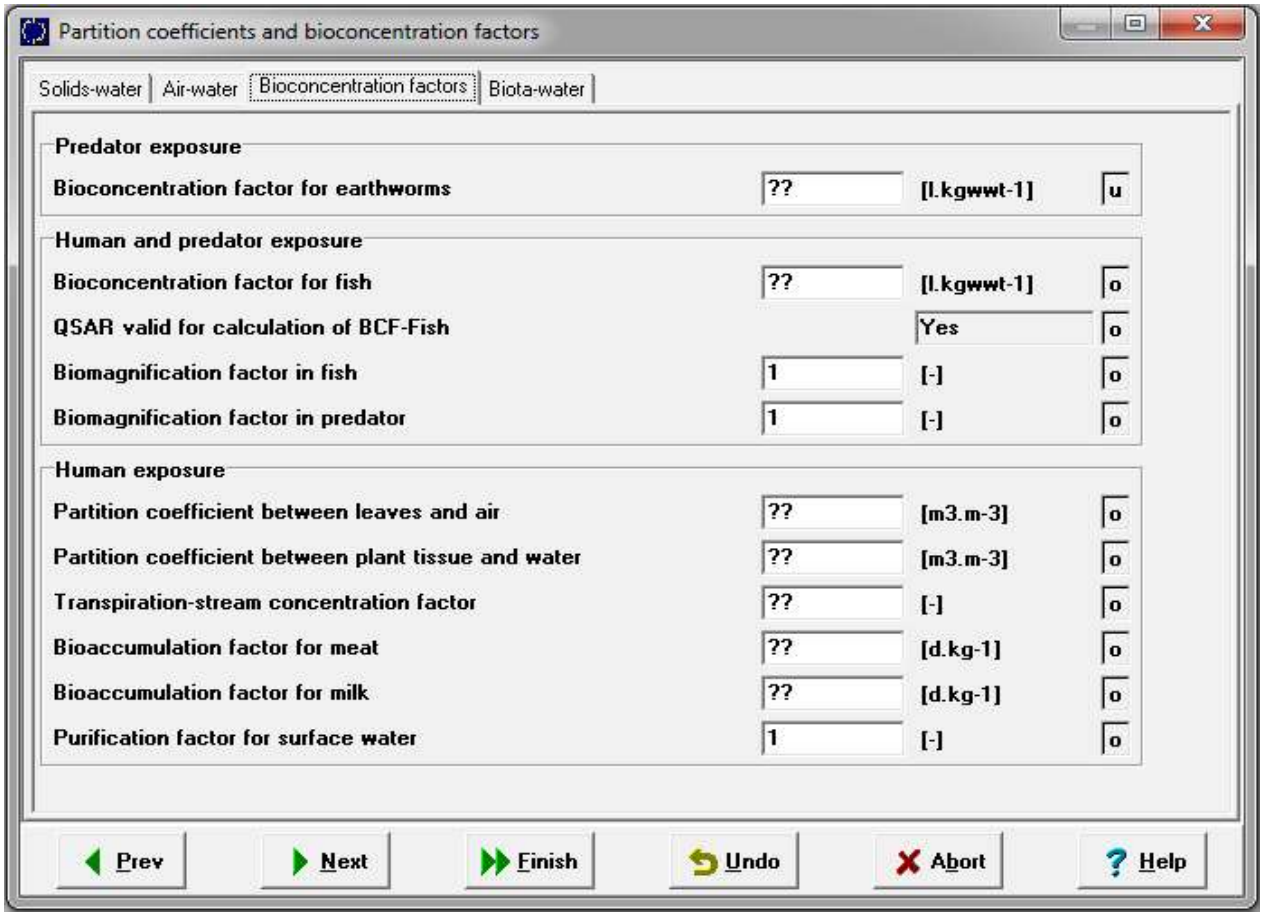
Current situation EUSES



Why needed?

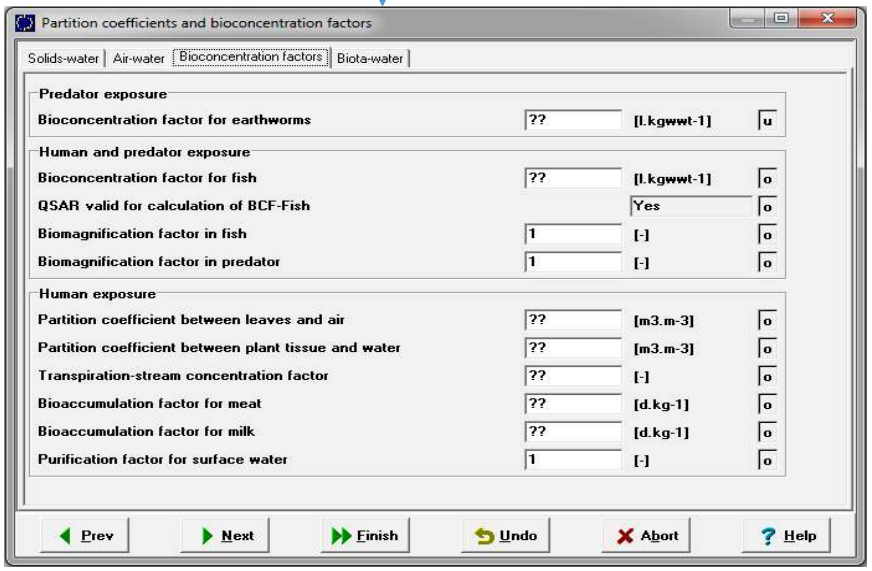
	Current EUSES
Organic, non-ionized, non-dissociating chemicals **(log Kow driven)**	• Plant leaves underestimated for hydrophilic compounds • Root crops are overestimated • Improved meat/milk estimation (biotransformation)
Ionized, dissociating chemicals (e.g. metals) **(not driven by log Kow)**	• Plants and roots: out of applicability domain

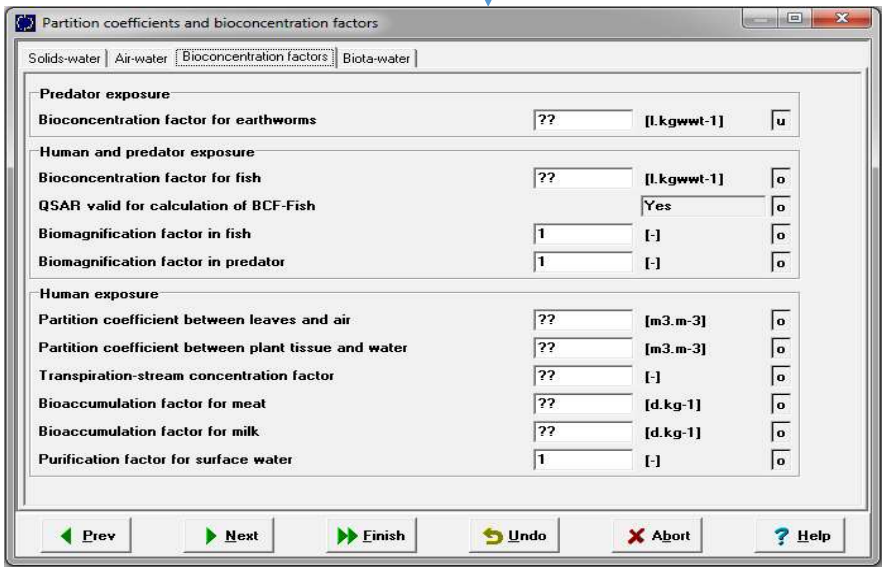
Change proposed

Kow driven?

yes

no



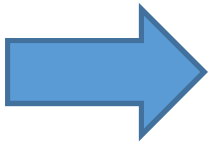


Change proposed (Kow driven)

- Plant leaves: update transpiration stream concentration factor

$$TSCF = 0.784 \cdot \exp\left[\frac{-(\log Kow - 1.78)^2}{2.44}\right]$$

Briggs et al. (1982)

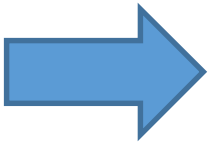


$$\mathrm{TSCF} = \frac{11}{11 + 2.6^{\log K_{ow}}}$$

Dettenmaier et al. (2009)

- Root crops: update model

$$C_{root} = \frac{K_{plant\text{-}water} \cdot C_{agric,porew}}{RHO_{plant}}$$



$$C_R = \frac{Q}{Q/K_{RW} + kV} C_S$$

Trapp (2002)

Change proposed (Kow driven)

- Meat/milk

$$BTF_{meat} = 10^{-7.6 + \log Kow} \text{ (log } K_{OW} \text{ range 1.5 to 6.5)}$$

$$BTF_{milk} = 10^{-8.1 + \log Kow} \text{ (log } K_{OW} \text{ range 3 to 6.5)}$$

Travis and Arms (1988)

(Franco et al., 2011)

Change proposed (not Kow driven)

- Allow user to input transfer factors
  - $TF_{roots,soil}$ is the dwt transfer factor from soil to roots (expressed in $kg_{soil}.kg_{roots}^{-1}$)
  - $TF_{leaves,soil}$ is the dwt transfer factor from soil to leaves (expressed in $kg_{soil}.kg_{leaves}^{-1}$)
  - $TF_{grass,soil}$ is the dwt transfer factor from soil to grass (expressed in $kg_{soil}.kg_{grass}^{-1}$)

Change proposed (not Kow driven)

- Model equations

$$C_{roots} = TF_{roots,soil} \cdot C_{soil}$$
$$C_{leaves} = TF_{leaves,soil} \cdot C_{soil}$$
$$C_{grass} = TF_{grass,soil} \cdot C_{soil}$$

Conclusions

MvE updates	Proposed priority
Organic, non-ionized, non-dissociating chemicals **(log Kow driven)**	Ready / important
Ionized, dissociating chemicals (e.g. metals) **(not driven by log Kow)**	Ready / important

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19 Secondary poisoning

Joost Bakker, RIVM

Current situation

To provide a first indication that secondary poisoning is a critical process three food chains are considered in EUSES:

Water (freshwater and marine environment) => fish => fish-eating predator

Water (marine environment) => fish => fish-eating predator => top-predator

Soil => earthworm => worm-eating predator

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Current situation

- For the freshwater and marine environment besides BCFs also biomagnification factors (BMF) must be applied.

- Default values for BMFs can either be based on the available log K_{ow} or BCF:

Log Kow $[m^3.m^{-3}]$	BCF (fish) $[m^3.kg_{wwt}^{-1}]$	BMF_1 [-]	BMF_2 [-]
< 4.5	< 2	1	1
4.5 - <5	2 – 5	2	2
5 - 8	> 5	10	10
>8 – 9	5 – 2	3	3
> 9	< 2	1	1

Proposed change

1.Modifying aquatic food chain by including an additional trophic level of piscivorous fish and considering fish feeding on plankton as proposed in the OSIRIS project:

Water => plankton => fish => piscivorous fish

Feeding on plankton can also contribute to bioaccumulation and potential biomagnification due extra trophic level is ignored in EUSES

Proposed change

2. Addition or Extension of terrestrial food chain:

Soil => earthworm => worm-eating predator => top-predator

To promote consistency in the risk assessment the same number of trophic levels as for the aquatic food chain is advocated

BMFs are required for terrestrial top-predators. BMF–Kow relationships or QSAR models needed.

Priority level

- Medium importance
  - Secondary poisoning particularly relevant for chemicals with log Kow 5-8
- Not ready
  - Proposal for aquatic food chain is documented and verified (OSIRIS proposal). Decide on how to fit in with current food chains in EUSES
  - For the terrestrial food chain default values for BMFs should be provided. Further research needed on availability and whether aquatic BMFs can be used in absence of terrestrial BMFs.

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20. Nanomaterials (chemicals in solid state/particulates)

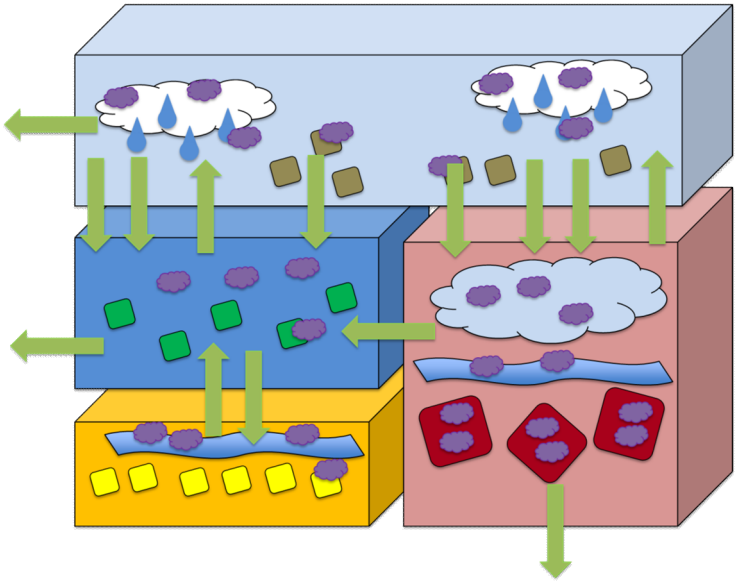
Joris Quik (RIVM)

National Institute for Public Health and the Environment
Ministry of Health, Welfare and Sport

Current situation in EUSES

- Distribution over gas, liquid and solid media by thermodynamic equilibrium (partitioning)
- Not applicable to nanomaterials/particulates

1. Thermodynamically unstable
2. Dissolution as removal
3. Transformation products



Proposed change (1)

Deposition

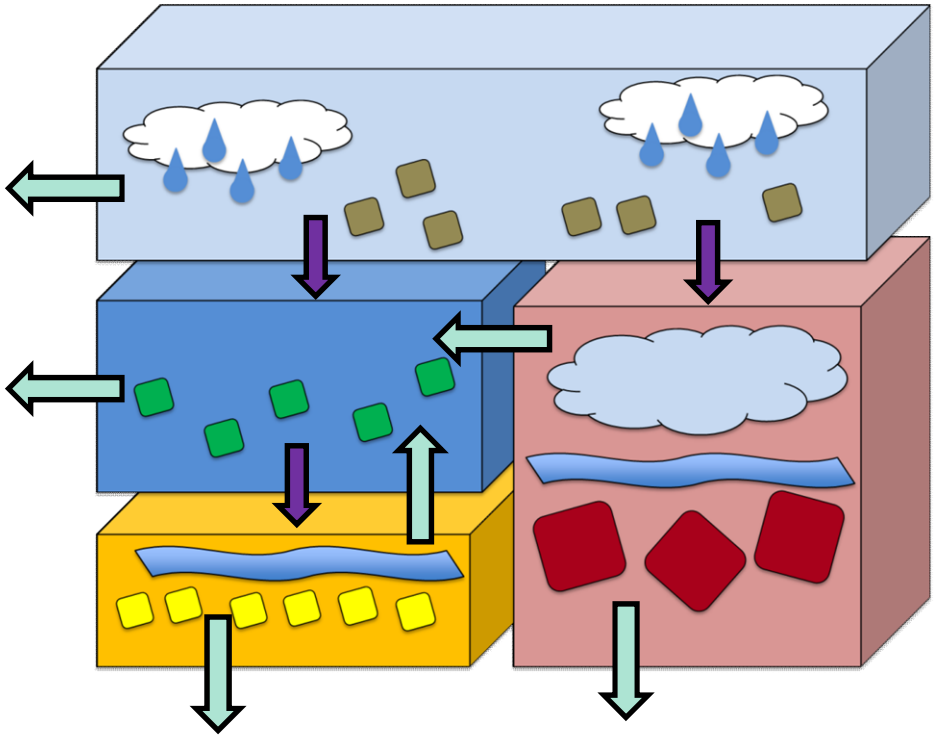
Dissolution

Attachment to natural particles

Use of process rate constants!

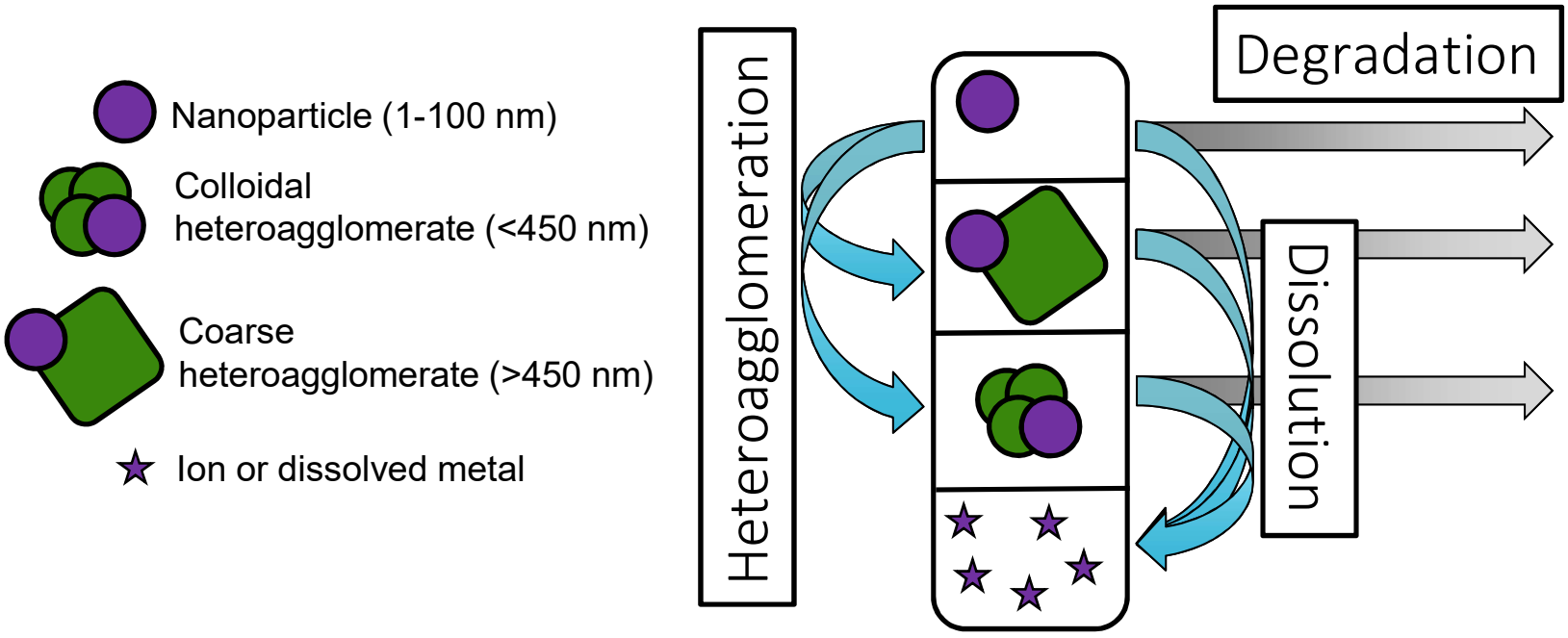
Proposed change (2)

- Transport processes
  - Deposition
  - Advection
  - No evaporation



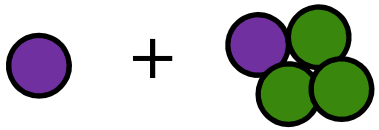
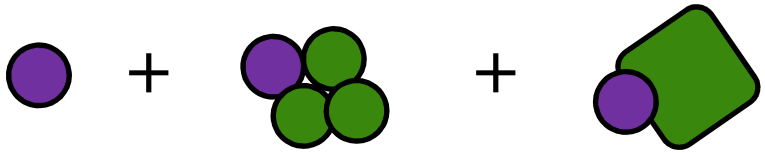
Proposed change (3)

- Transformation processes included:



Proposed change

Output concentrations:

- Free: 
- Bioavailable:  (< 450 nm)
- Total: 
- Dissolved: ★ is no longer nanomaterial

Priority level

- High importance
  - Technically ready with respect to fate modelling of nanomaterials at regional scale
  - Modelling approach facilitates other improvements:
    - Metal species and microplastics
  - REACH Annexes adapted for nanomaterials
    - Indicating specific requirements, come into effect 1-1-2020
  - Not ready for implementation
    - Related to other EUSES modules: emission, local scale, etc

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21. Release and fate of sparingly soluble chemicals

Joris Quik (RIVM)

Current status in EUSES

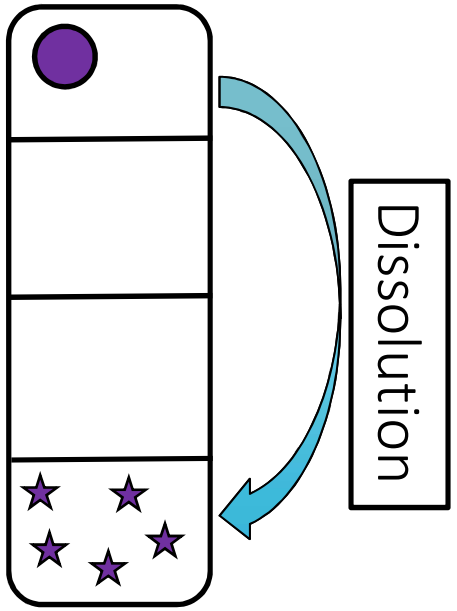
- Enable EUSES to consider in the exposure estimation the dissolution of solid substances.
- This particularly affects substances emitted in solid form, particularly metals

Proposed change/way forward

- Dissolution rate constant

Nanoparticle (1-100 nm)

Ion or dissolved metal



Priority level

- Suggested priority: Not ready/ low importance
  - Affects all sparingly soluble chemicals
  - Proposed method similar to implementation for nanomaterials
  - Impact on exposure can be large.
  - New data requirement
    - OECD 29 (7 days) for metals is not directly a testing requirement but can replace the water solubility endpoint for metals and metal compounds.
    - Other OECD TG's in development for estimating dissolution rate in relation to nanomaterials.

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22-24 Metals

Anna Hadam
Frederik Verdonck

Gaps for metals

Current situation in EUSES	Problems identified for metals
Primarily developed for neutral organic substances	Numerous inadequate assumptions for metals
Only the total dissolved and particulate fractions Kd values: calculated based on the log Kow independent on the environmental chemistry	Overestimation of the actual (bio)availability and toxicity Kd measured values needed posteriori bio-availability correction outside EUSES (for both PECs and PNECs)
Mackay level III model	Longer-term / additional specific fate processes not taken into account
No possibilities for the Added Risk Approach	Manual calculations outside EUSES

Content

- metals bioavailability
- PECs refinement
- metal-specific fate processes
- natural background concentration

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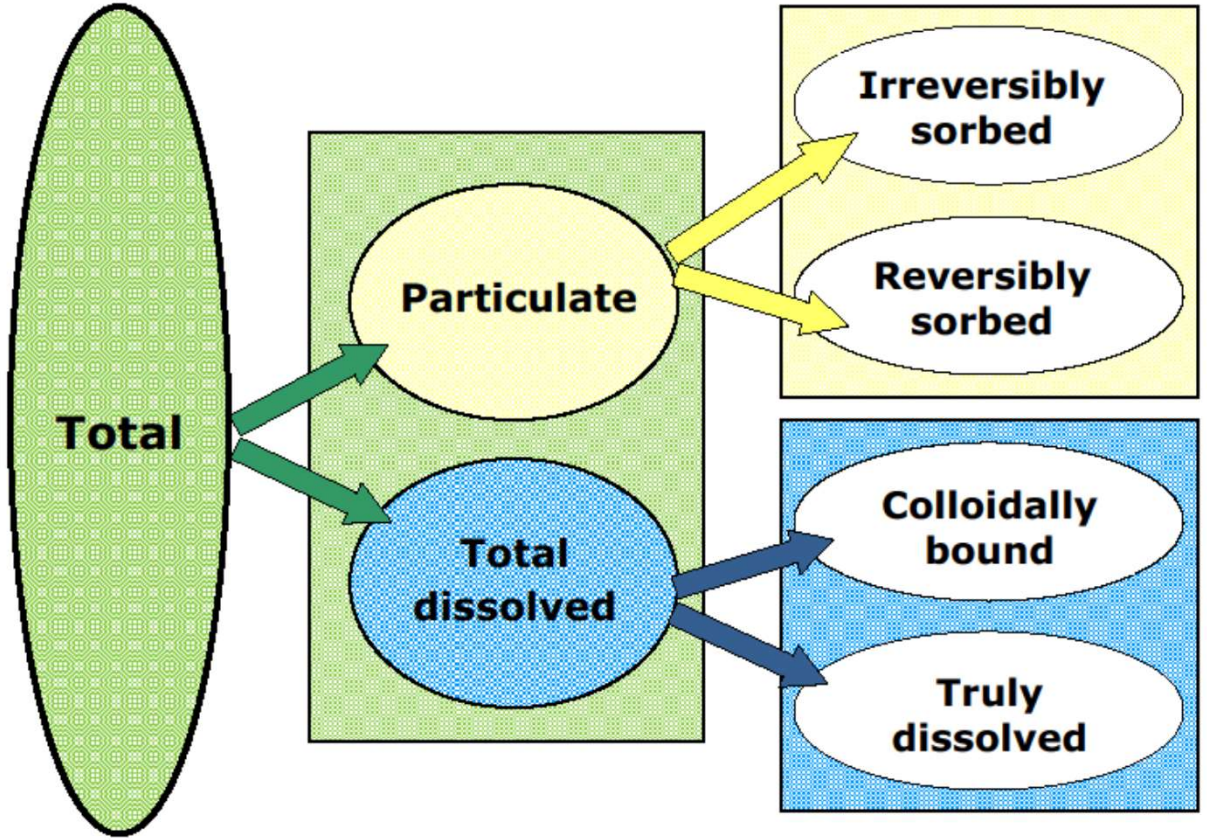
Truly dissolved form

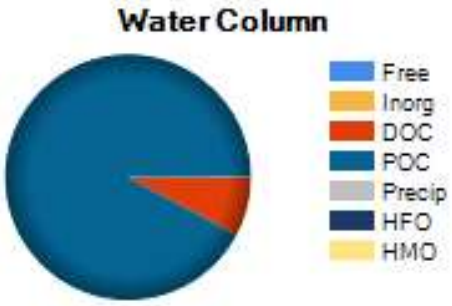
- (e.g.) WHAM



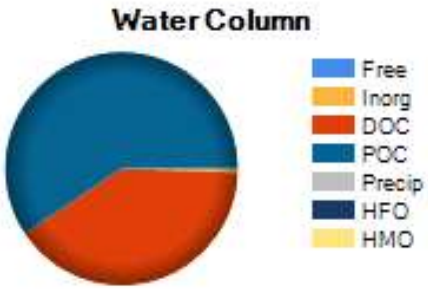
- Site-specific chemical conditions (pH, DOC, cations & anions …)

Ecoregion impact on Cu speciation in surface water

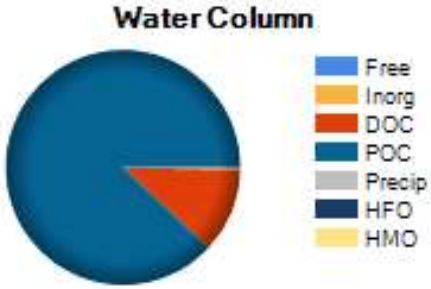
- **UWM euses lake**



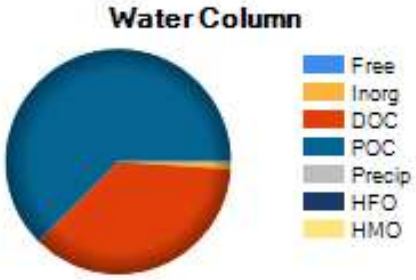
- **Terne – UK**



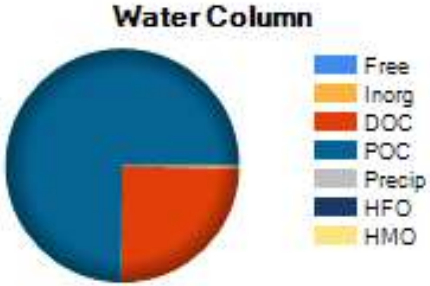
- **Monate – IT**



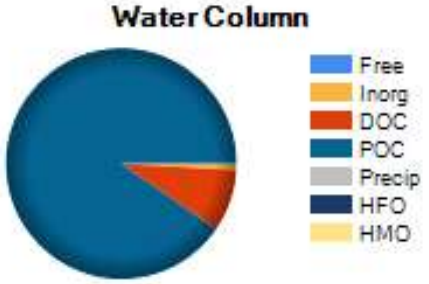
- **Ditch – NL**



- **Rhine – NL**



- **Lake – Sw**



Impact of Kd on exposure

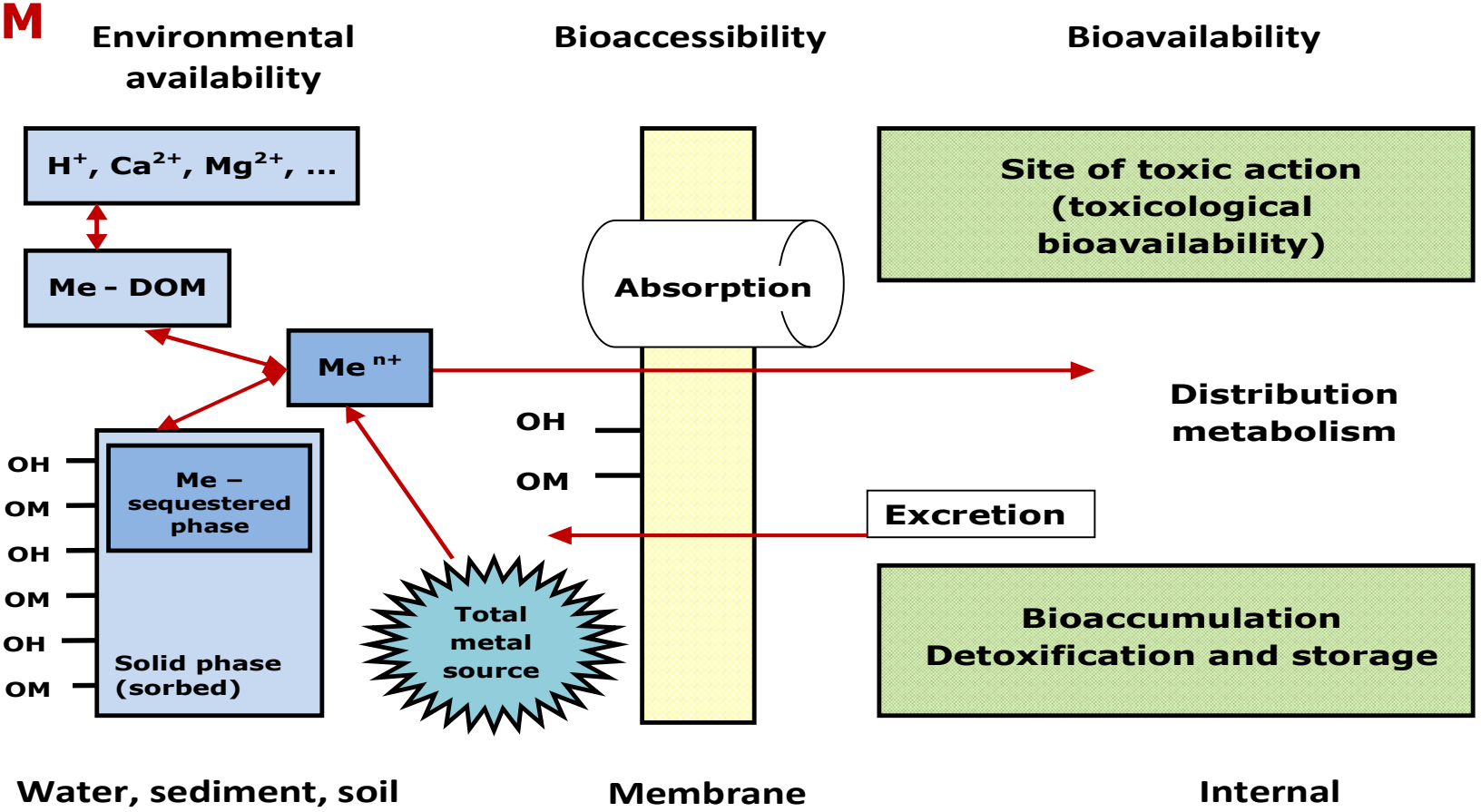
- Big impact on dissolved water concentration

EUSES	PEC freshwater		PEC sediment
	Total (ug/L)	Dissolved (ug/L)	Total (ug/kg wwt)
Cu Kd, suspended matter			
10th percentile = 5,752 L/kg	0.25	0.23	516
50th percentile = 30,246 L/kg	0.15	0.1	1209
90th percentile = 194,228 L/kg	0.08	0.02	1653

- **10x**

Bioavailability concept

- **BLM**



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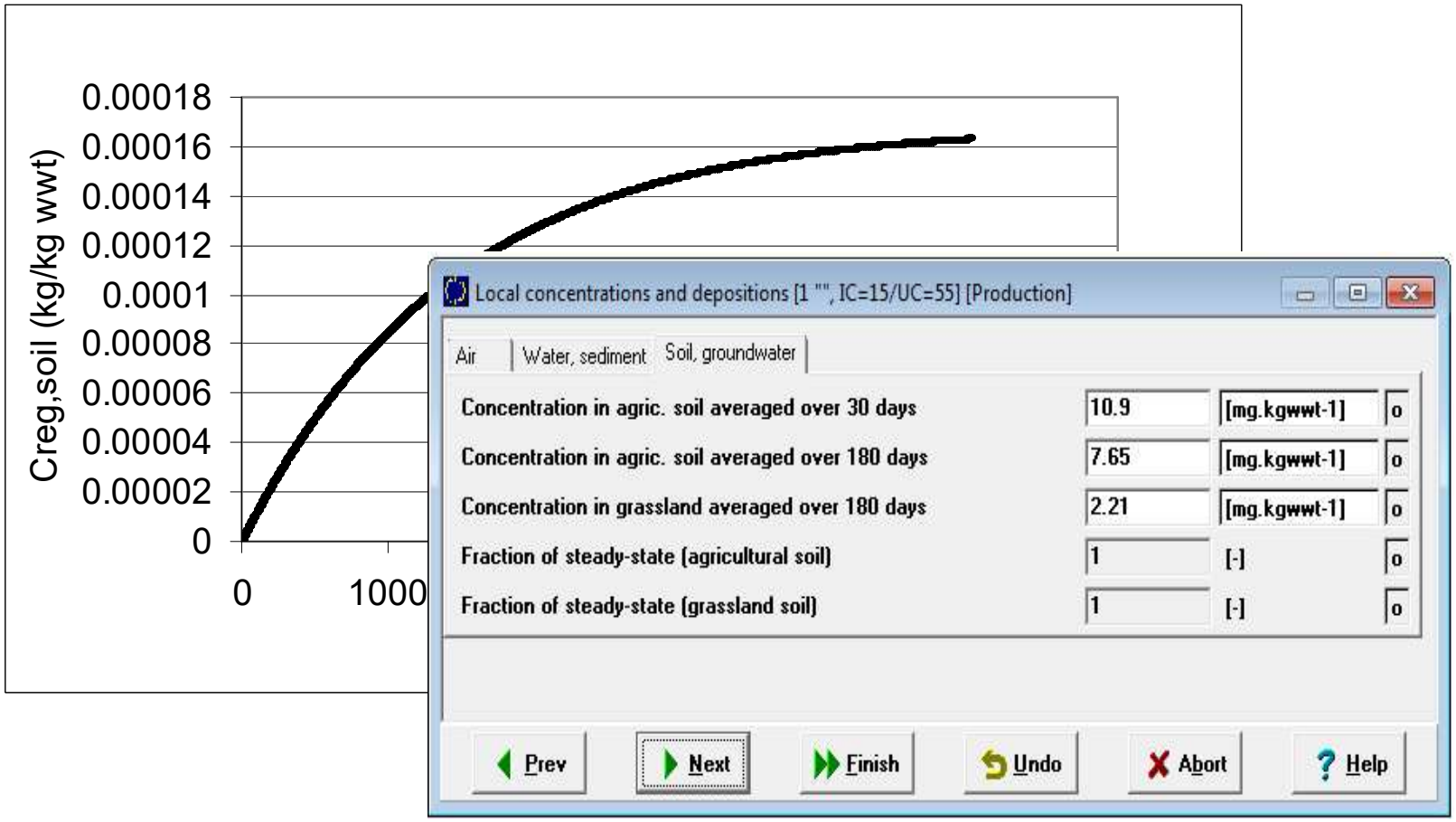
PECs refinement (regional scale)



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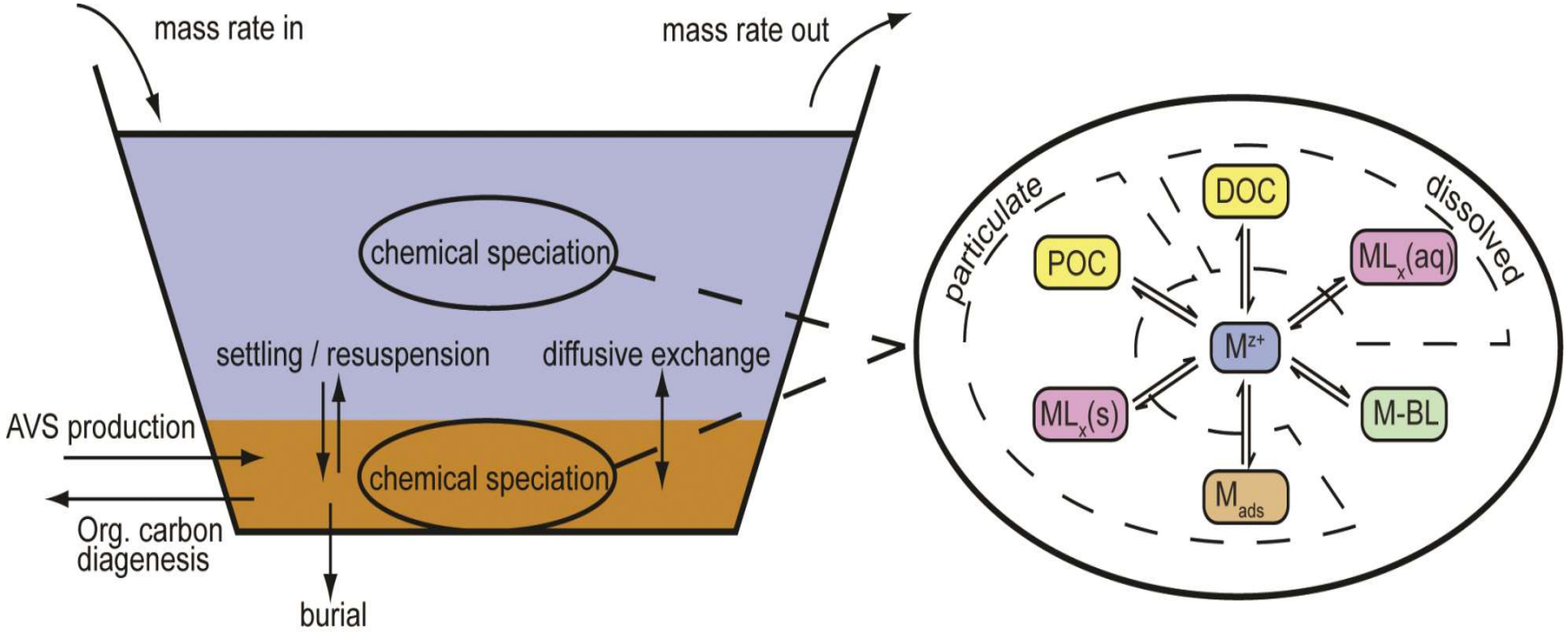
Comparison metal fate and transport processes

	EUSES	TICKET-UWM
adsorption to particulate organic carbon (POC)	**(X)**	**X**
dissolved and particulate phase transport between water and sediment	**X**	**X**
metal binding to inorganic ligands, DOC and POC (using WHAM V), hydrous ferric oxide (HFO) and hydrous manganese oxide (HMO)	**(X)**	**X**
metal binding to biological receptors (using BLM)		**X**
metal precipitation as (hydr)oxides, carbonates and sulphides (using MINEQL+)		**X**
dissolution kinetics for metal powders, massives, etc.		**X**
average annual cycling of organic matter and sulphide production		**X**

Additional metal-specific fate processes

- **TICKET – UWM »»» water and sediment**



- **metal binding, metal precipitation, dissolution kinetics, cycling of organic matter, sulphide production**

Additional metal-specific fate processes

- **IDMM»»»» soil**

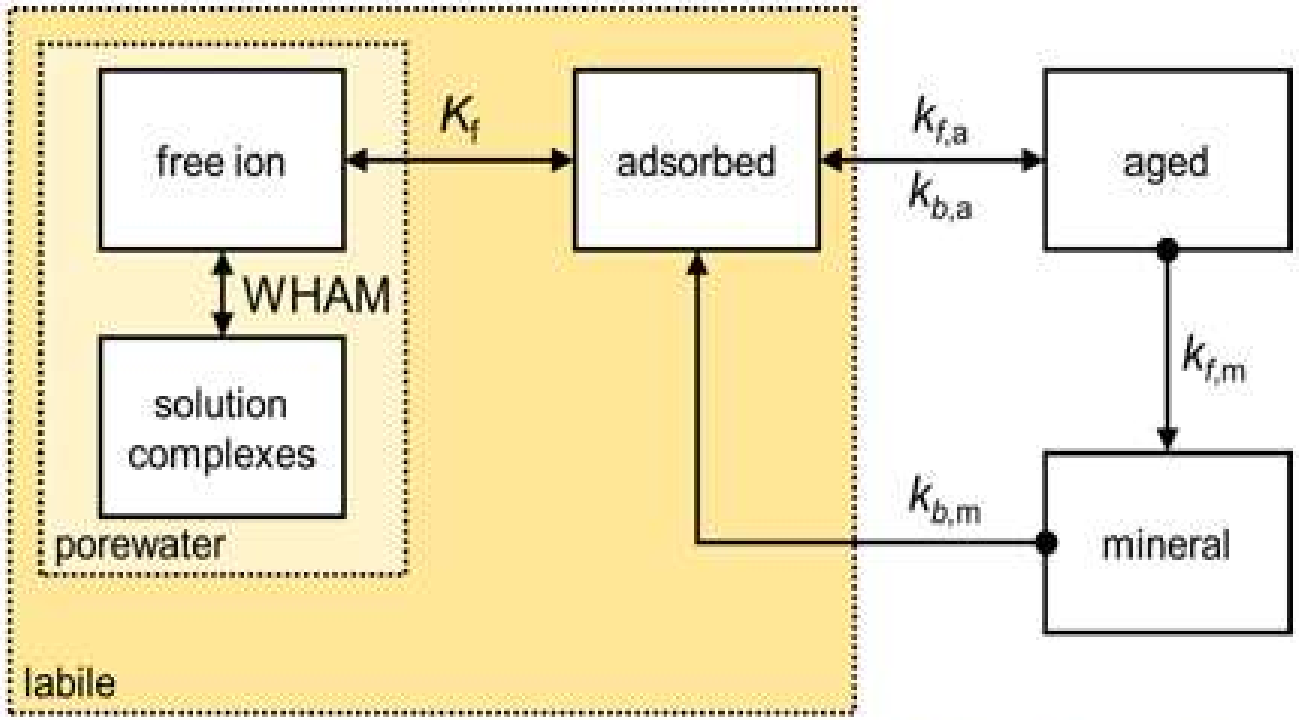


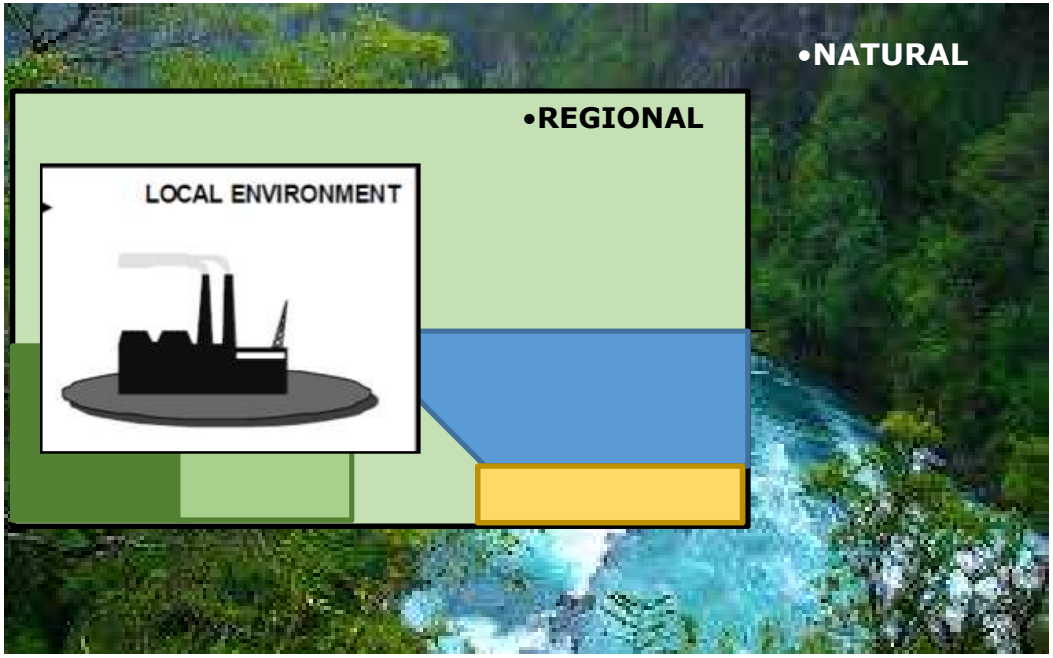
Figure 2. Schematic diagram of metal transformations in soils. Large K denotes an equilibrium transformation parameter, small k denotes a kinetic transformation parameter.

Natural background concentration

- **Total Risk Approach**

•PEClocal $_{compartment,\ total}$ =

•PEClocal $_{compartment,\ added}$ + PECregional $_{compartment}$ + PEC natural/pristine $_{compartment}$



Conclusions

Proposed change	Proposed priority
Bioavailability concept	Not ready (long-term project) Highly important
PECs refinement	Ready Highly important
Additional fate processes	Not ready (long-term project) Highly important
Natural background concentration	Ready Highly important

Considerations for the future

- choice of the average /worst-case biochemical regions for each kind of metal/ in the UE (representative pH, DOC, alkalinity, etc. of the environmental compartments; number of representative regions);
- validation and agreement on the choice of geochemical speciation (e.g. WHAM) and BLM models;
- method of EUSES update (Kp and PNEC values derivation outside EUSES or implementation of the agreed tools into EUSES)
- addition of long-term metal mineralisation (insolubilization) fate process

FS1

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25. Parallel assessment (for multi-constituent substances and for substances transforming on use/ in STP)

Heike Schimmepfennig

Slide 54

FS1 just few little correction to you draft

FRATTINI Stefano, 29/05/2018

Current situation in EUSES

- Hydrocarbon Block Method (HBM) module
  - enables parallel exposure and hazard assessments of defined “blocks”.
  - developed to support the assessment of multi-constituent chemicals (initially hydrocarbons)
- Locked for biocides assessment on local scale!

Proposed change (1)

- Parallel assessment concept applicable to other cases than hydrocarbons:
  - Assessment of multi-constituents chemicals (or UVCBs)
  - Assessment of several substances part of a mixture
  - Assessment of substance and its transformation product
- Similar to risk assessment approach implemented in Chesar (for REACH)
  - "Assessment Entities" for multi-constituent/UVCB substances and transformation products
  - Logic in line with HBM module

Proposed change (2)

- Functioning of assessment entities in Chesar
  - Introducing separate properties data sets => Data sets of various constituents of a substance or transformation product(s) and/or parent substance
  - Proportion for each element to be set by assessor

→HBM module in EUSES to be used in same way

  - Note: static parallel assessment only possible where no temporal variations taken into account

Proposed way forward

- Unlock HBM for biocides and adapt it to biocides specific emission estimation
- Rename it more generically to reflect its usability for UVCB substances, mixtures, etc. falling under REACH and biocides regulations

Priority level TE4

- High importance
  - Possibility for parallel exposure/risk assessment not available for biocides assessment
  - Assessment of multi-constituent and UVCB substances, mixtures, several active substances/substances of concern in biocidal products, parent substance and transformation products (or substances generated in situ with precursors) legally required
  - **Ready for implementation**

Slide 59

TE4 shall we present the suggested priority level using the same structure as described in the introduction BD and Anna's presentation ?
TSITSIOU Eleni, 30/05/2018

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26. Assessment of substance transforming in the environment

Heike Schimmelpfennig

Current situation in EUSES

- No module available in EUSES enabling exposure/risk assessment for transformation products and/or parent substance, taking into account degradation/transformation processes
  - As e.g. implemented in FOCUS models (PEARL, PELMO, GOCUS Surface water)

Proposed change/way forward

- Explore the need for refining the assessment methods when substances are transformed in the environment for REACH substances and biocides
- Information available
  - Multi-species mass balance modelling implemented by Van Zelm et al. (2008)
  - OSIRIS project, documented by Ng et al. (2011)

Priority level

- Medium importance
  - Need for further validation of available principles and methodology of modelling + regulatory relevance and acceptance of it needs
  - Update would affect limited number of substances transforming in the environment into products of concern
  - **Not ready for implementation**

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27. Aggregate local exposure assessment (biocides)

Heike Schimmelpfennig

Current situation

- BPR: Within the process of evaluation of dossiers for biocidal products, possibility of aggregated exposure must be taken into account (BPR Annex VI, Article 8(3) and Article 19, 2(c))
  - Specific guidance currently under preparation, decision tree already available
- EUSES: Exposure assessments for biocides per single use => aggregated exposure assessment performed outside EUSES

Proposed change/way forward

- Implement in EUSES possibility to assess several uses for same active substance in one assessment (within one PT + between different PTs)
- Note: Chesar already supports local assessment of sum of all widespread uses
  - But: simultaneous use at a given site not yet supported in current Chesar version

Priority level

- High importance
  - for biocides according to ECHA
  - reservations from ECETOC
  - **Nearly ready for implementation**

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Thank you!