Task Force
Sufficiency of aquatic hazard information for environmental risk assessment

Topical Scientific Workshop on Soil Risk Assessment

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2. General methods - Data collection and cleanup
3. Methods, Results & Discussion
   a) Hazard comparison (I) - Direct comparison
   b) Hazard comparison (II) - Role of phys-chem & MOA
   c) Hazard comparison (III) - Chemical activity
   d) How significant is all of this in a risk assessment? - PNEC comparison
4. Conclusions & Suggestions

Background

- REACH ecotoxicological data requirements
  - 1 to 10 t/yr: only acute aquatic data
  - 10 to 100 t/yr: only acute aquatic data
  - 100 to 1000 t/yr: chronic aquatic and acute terrestrial data
    => EqP can be used if no data available
  - > 1000 t/yr: chronic terrestrial included

→ Environmental hazard and risk assessments under REACH depend strongly on aquatic ecotoxicity data

Background

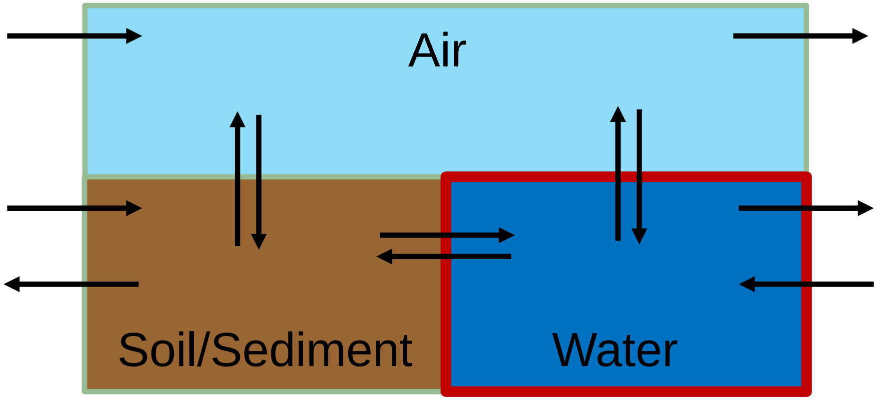
- REACH **aquatic** hazard and risk assessment
  - What's the hazard for aquatic species?
    $\rightarrow$ $PNEC_{aquatic}$ = 0,025 mg/L

EC50 (mg/L)	25	32	> 100

$$\frac{25\,\text{mg/L}}{\text{AF}} = \frac{25\,\text{mg/L}}{1000} = 0.025\,\text{mg/L}$$

  - To what levels are aquatic species exposed?
    $\rightarrow$ $PEC_{aquatic}$ = 0,005 mg/L

$$RCR = \frac{PEC_{aquatic}}{PNEC_{aquatic}} = \frac{0.005}{0.025} = 0.2$$



Background

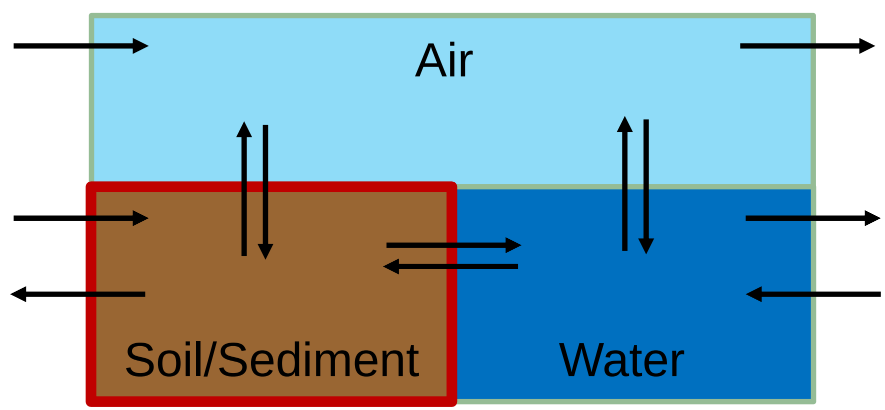
- REACH **soil** hazard and risk assessment - option A
  - What's the hazard for soil species?
    $\rightarrow PNEC_{soil,AF} = 0{,}264$ mg/kg

$$\frac{264 \text{ mg/kg}}{AF} = \frac{264 \text{ mg/kg}}{1000} = 0.264 \text{ mg/kg}$$

EC50 (mg/kg) 264

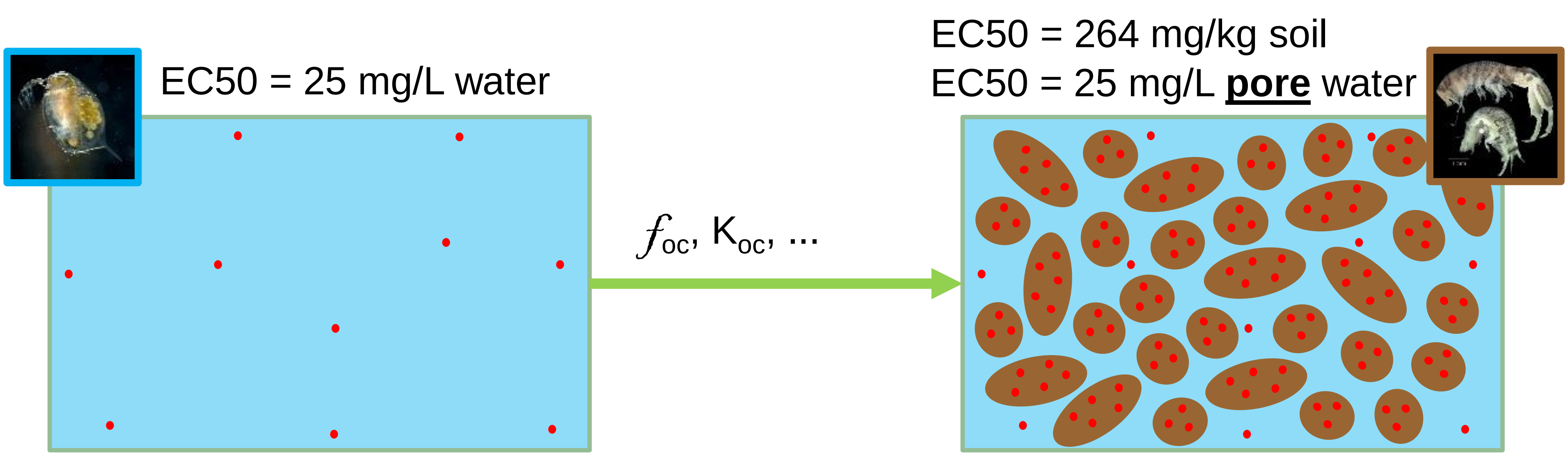
  - To what levels are soil species exposed?
    $\rightarrow PEC_{soil} = 0{,}05$ mg/kg

$$RCR = \frac{PEC_{soil}}{PNEC_{soil,AF}} = \frac{0.05}{0.264} = 0.2$$



Background

- REACH **soil** hazard and risk assessment - option B
  - What's the hazard for soil species?
    → $PNEC_{soil}$ derived from $PNEC_{aquatic}$ using equilibrium partitioning (**EqP**)
    - Aquatic and soil organisms are equally sensitive
    - Toxicant uptake via water phase



Background

REACH **soil** PNEC derivation

Option A
- Experimental soil EC50
- Assessment factor (AF)

Option B
- Experimental aquatic EC50
- Equilibrium partitioning (EqP)

$PNEC_{soil,AF}$? = $PNEC_{soil,EqP}$

Do we miss any risks when using $PNEC_{soil,EqP}$?

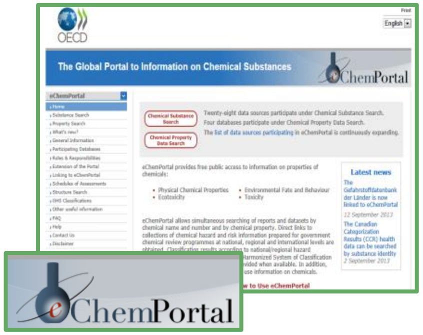
Terms of reference (excerpt)

ecetoc

- Confirm the **extent** to which the existing sys… describing the **aquatic hazard** of subst… **protective** for risks in the compart… …er, soil, and sediment.
- Identify those substan… …r which a **better understanding** m… …quired.
- Review a… …ormation acquisition strategies for obtai… …d information in soil and sediment with th… **identifying reliable approaches** for …ving the confidence in the environmental safety assessment.

Exercise with a regulatory focus!

Data mining



eChem Portal

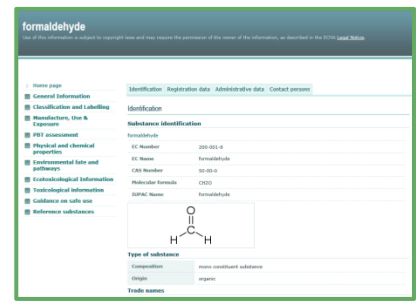
Develop a database containing substances with:

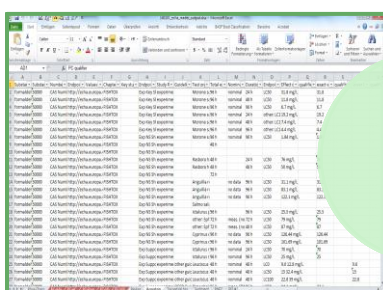
- Aquatic and terrestrial (soil) toxicity data
- (Aquatic and sediment toxicity data)

~ **500 substances** have been identified carrying both aquatic and terrestrial data (Klimisch score 1 & 2 only).

Additional data extracted from ECHA webpage: **Phys-Chem**, **biodegradation, PNECs**

ECHA website



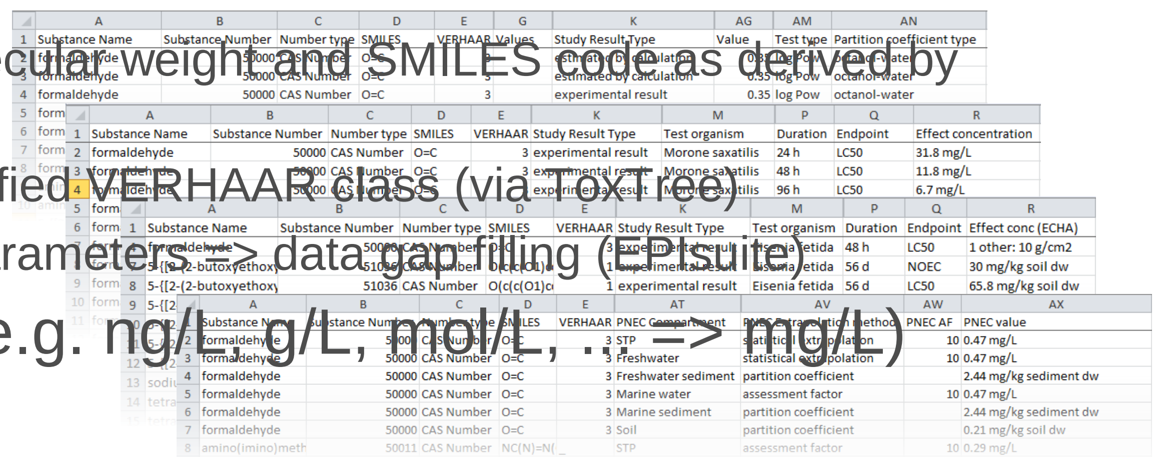


xlsx

The list covers **12 182 endpoint study records**.

Data mining

- Ecotoxicity data, acute and chronic
  - Aquatic: algae (& other aquatic plants), invertebrates and fish; PNECs
  - Terrestrial: plants, soil dwelling organisms, soil microorganisms; PNECs
  - Phys-Chem data: Kow, Koc, Vapour pressure, Henry's law constant, water solubility
- Data cleanup: units, endpoints, exposure duration, ...
- Additions
  - Chemical class, molecular weight and SMILES code as derived by ECOSAR
  - Mode of action: Modified VERHAAR class (via ToxTree)
  - QSAR phys-chem parameters => data gap filling (EPIsuite)
- Unit conversions (e.g. ng/L, g/L, mol/L, ... => mg/L)



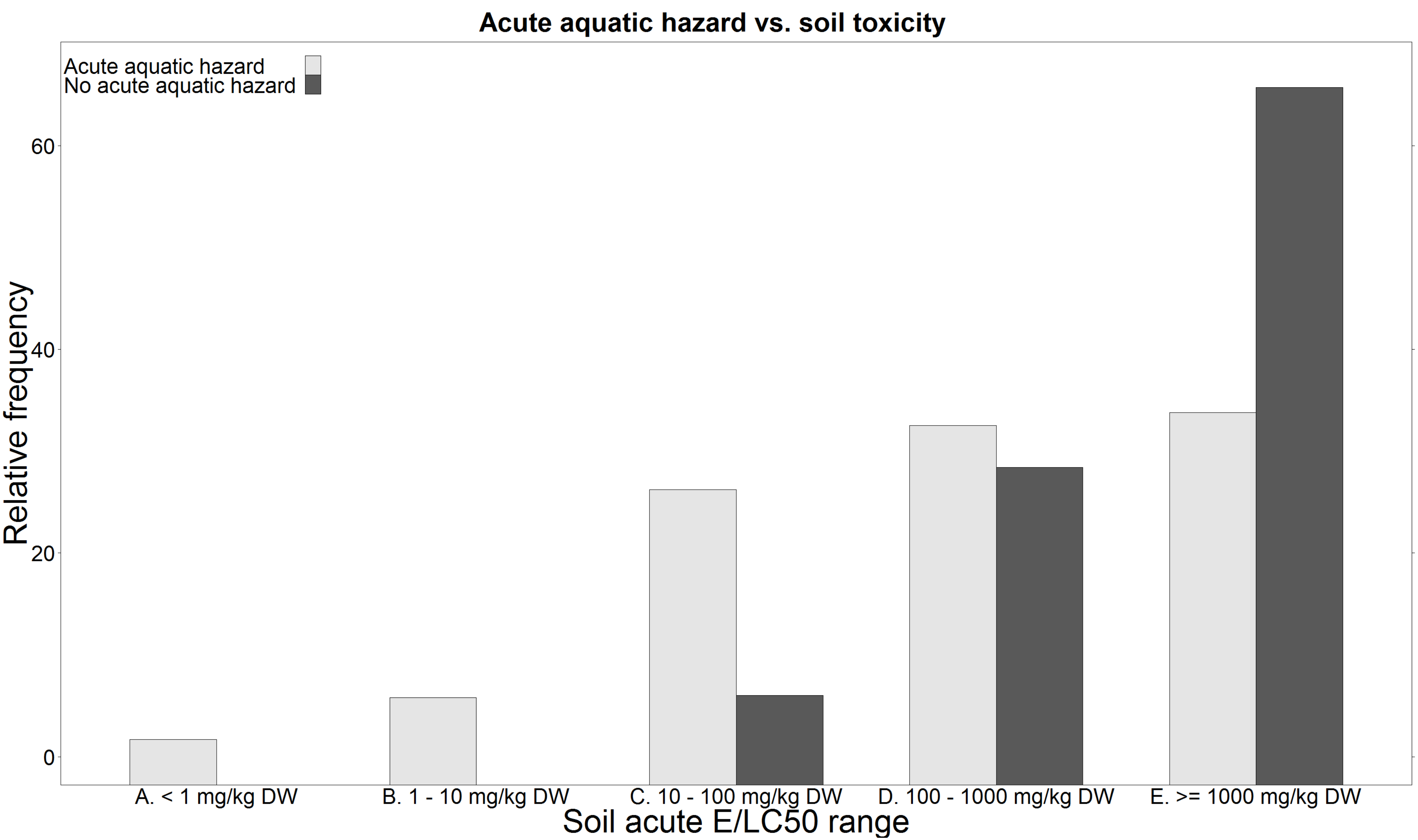
Substance Name	Substance Number	Number type	SMILES	VERHAAR Values	Study Result Type	Value	Test type	Partition coefficient type
formaldehyde	50000	CAS Number	O=C	3	estimated by calculation	[illegible]	log Pow	octanol-water
formaldehyde	50000	CAS Number	O=C	3	estimated by calculation	0.35	log Pow	octanol-water
formaldehyde	50000	CAS Number	O=C	3	experimental result	0.35	log Pow	octanol-water

Substance Name	Substance Number	Number type	SMILES	VERHAAR	Study Result Type	Test organism	Duration	Endpoint	Effect concentration
formaldehyde	50000	CAS Number	O=C	3	experimental result	Morone saxatilis	24 h	LC50	31.8 mg/L
formaldehyde	50000	CAS Number	O=C	3	experimental result	Morone saxatilis	48 h	LC50	11.8 mg/L
formaldehyde	50000	CAS Number	O=C	3	experimental result	Morone saxatilis	96 h	LC50	6.7 mg/L

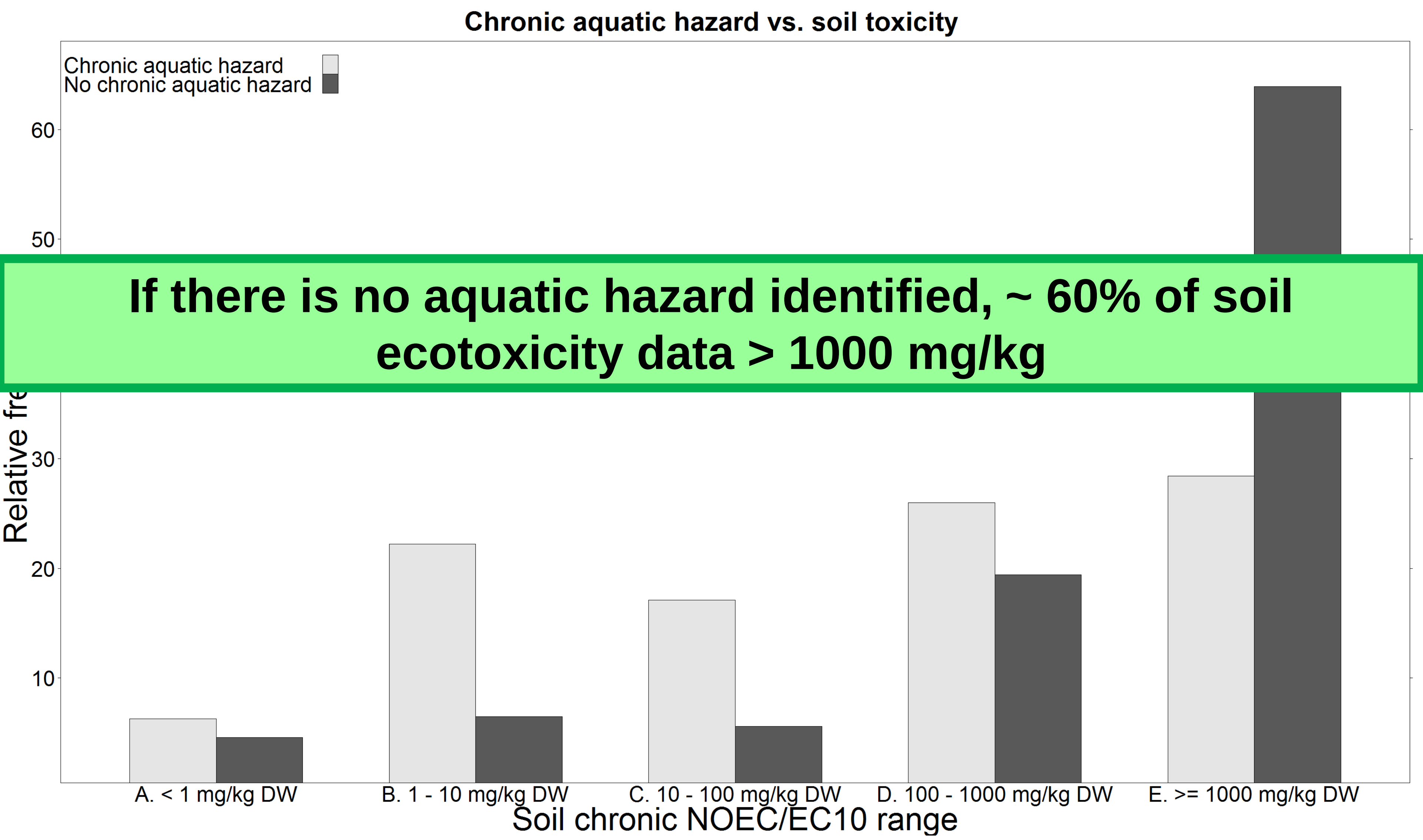
Substance Name	Substance Number	Number type	SMILES	VERHAAR	Study Result Type	Test organism	Duration	Endpoint	Effect conc (ECHA)
formaldehyde	50000	CAS Number	O=C	3	experimental result	Eisenia fetida	48 h	LC50	1 other: 10 g/cm2
5-{[2-(2-butoxyethoxy	51036	CAS Number	O(c(c(O1)c	1	experimental result	Eisenia fetida	56 d	NOEC	30 mg/kg soil dw
5-{[2-(2-butoxyethoxy	51036	CAS Number	O(c(c(O1)c	1	experimental result	Eisenia fetida	56 d	LC50	65.8 mg/kg soil dw

Substance Name	Substance Number	Number type	SMILES	VERHAAR	PNEC Compartment	PNEC Extrapolation method	PNEC AF	PNEC value
formaldehyde	50000	CAS Number	O=C	3	STP	statistical extrapolation	10	0.47 mg/L
formaldehyde	50000	CAS Number	O=C	3	Freshwater	statistical extrapolation	10	0.47 mg/L
formaldehyde	50000	CAS Number	O=C	3	Freshwater sediment	partition coefficient		2.44 mg/kg sediment dw
formaldehyde	50000	CAS Number	O=C	3	Marine water	assessment factor	10	0.47 mg/L
formaldehyde	50000	CAS Number	O=C	3	Marine sediment	partition coefficient		2.44 mg/kg sediment dw
formaldehyde	50000	CAS Number	O=C	3	Soil	partition coefficient		0.21 mg/kg soil dw
amino(imino)meth	50011	CAS Number	NC(N)=N(		STP	assessment factor	10	0.29 mg/L
amino(imino)meth	50011	CAS Number	NC(N)=N(		Freshwater	assessment factor	10	0.29 mg/L

Hazard comparison (I) – Direct comparison



Hazard comparison (I) – Direct comparison



If there is no aquatic hazard identified, ~ 60% of soil ecotoxicity data > 1000 mg/kg

Hazard comparison (II) – Role of phys-chem & MOA

- Unit conversion
  - mg/kg dry (or wet) weight => mg/L pore water
  - Equilibrium partitioning method (EPM; formulas from ECHA guidance)
- Why EPM?
  - Comparability of units
  - No hazard threshold for soil
  - The concept makes sense and offers a good basis for this exercise => in which cases does the hazard to soil and sediment organisms deviate from what EP theory would predict?

Hazard comparison (II) – Role of phys-chem & MOA

- Data presentation

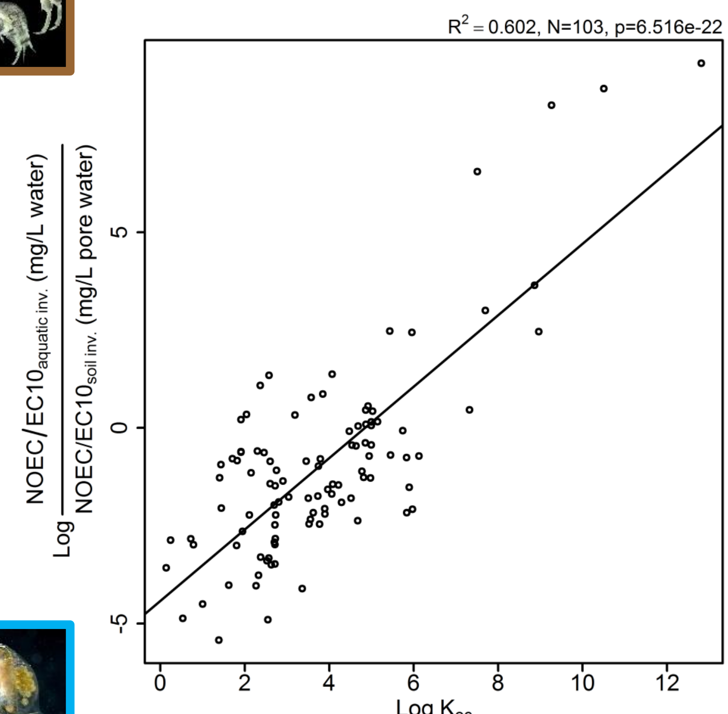
$$\text{Log}\ \frac{\text{EC50}_{\text{aqua,inv}}}{\text{EC50}_{\text{soil,inv}}}$$

$> 0 \rightarrow \text{EC50}_{\text{aqua,inv}} > \text{EC50}_{\text{soil,inv}}$

$\rightarrow$ Soil invertebrates are more sensitive

$< 0 \rightarrow \text{EC50}_{\text{aqua,inv}} < \text{EC50}_{\text{soil,inv}}$

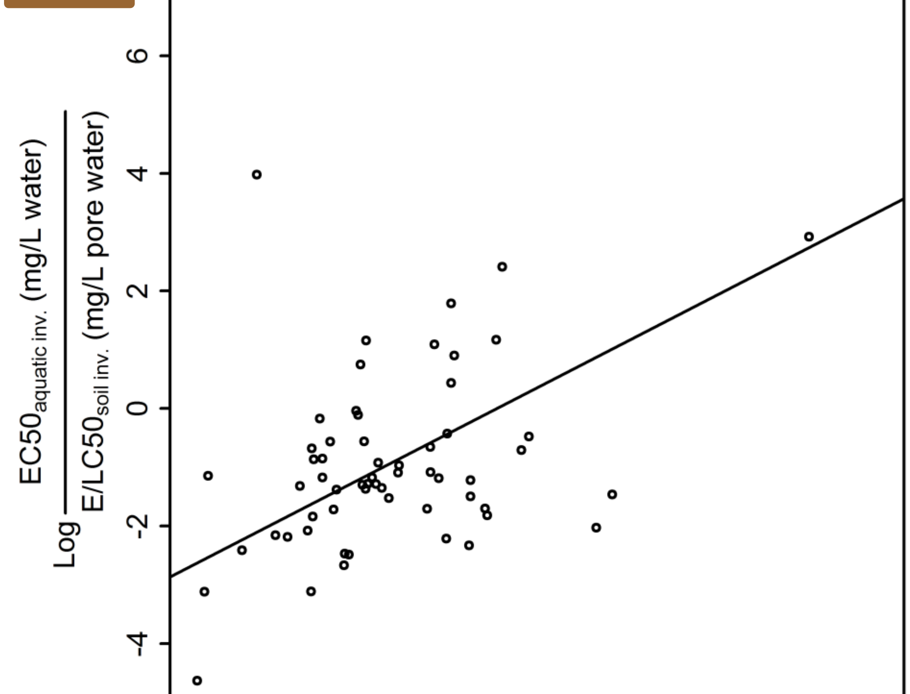
$\rightarrow$ Soil invertebrates are less sensitive

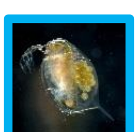


Hazard comparison (II) – Role of phys-chem & MOA

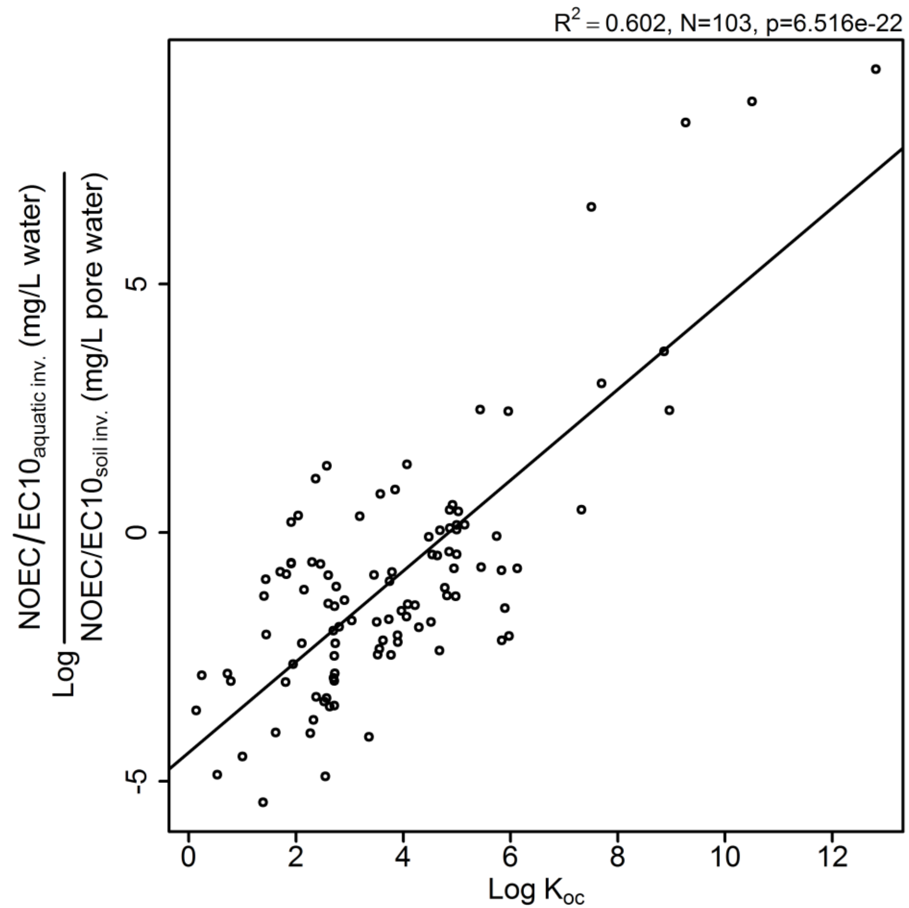
PC - Versus Log Koc (aquatic vs soil invertebrates)

Acute





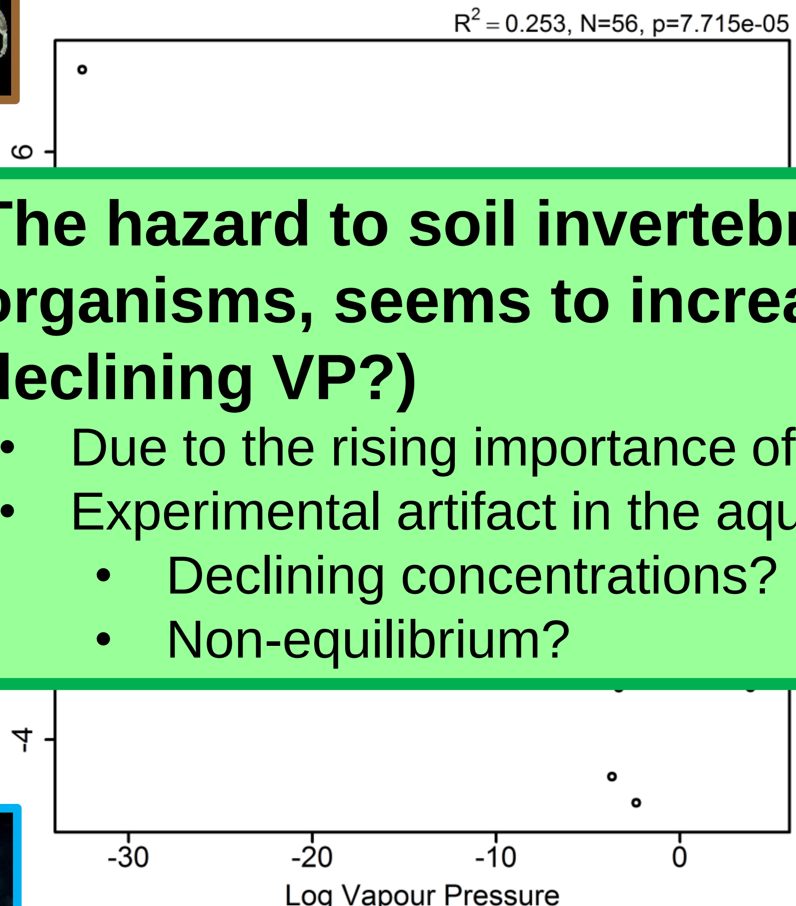
Chronic



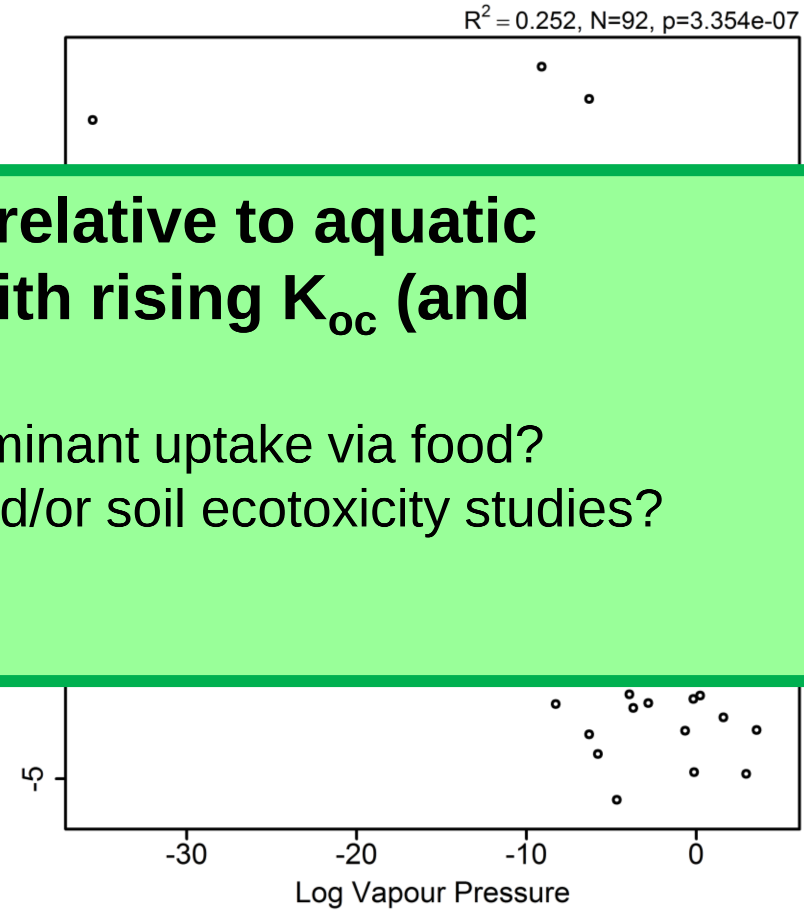
Hazard comparison (II) – Role of phys-chem & MOA

PC - Versus Log VP (aquatic vs soil invertebrates)

Acute



Chronic

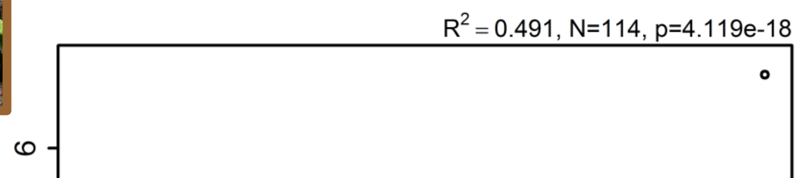


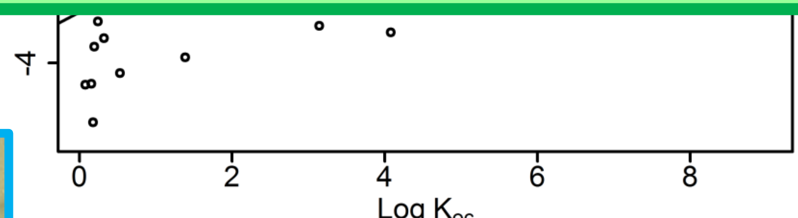
- **The hazard to soil invertebrates relative to aquatic organisms, seems to increase with rising K_{oc} (and declining VP?)**
  - Due to the rising importance of contaminant uptake via food?
  - Experimental artifact in the aquatic and/or soil ecotoxicity studies?
    - Declining concentrations?
    - Non-equilibrium?

Hazard comparison (II) – Role of phys-chem & MOA

PC - Versus Log Koc (Algae vs terrestrial plants)

Acute





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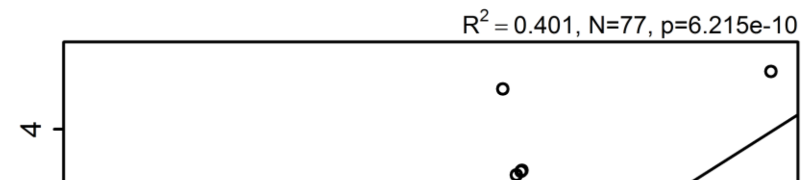
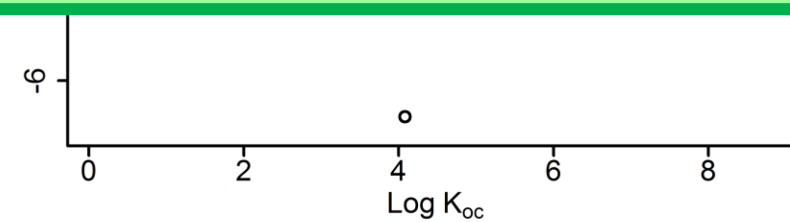


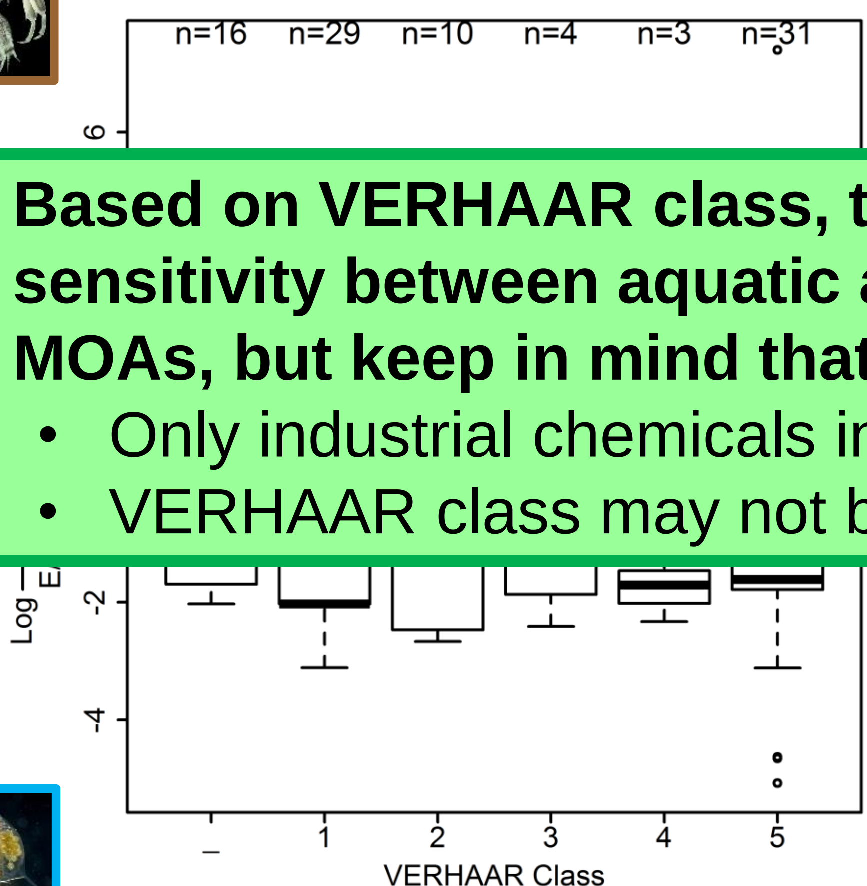


- **The hazard to soil invertebrates relative to aquatic organisms, seems to increase with rising K_{oc} (and declining VP?)**
  - Due to the rising importance of contaminant uptake via food?
  - Experimental artifact in the aquatic and/or soil ecotoxicity studies?
    - Declining concentrations?
    - Non-equilibrium?

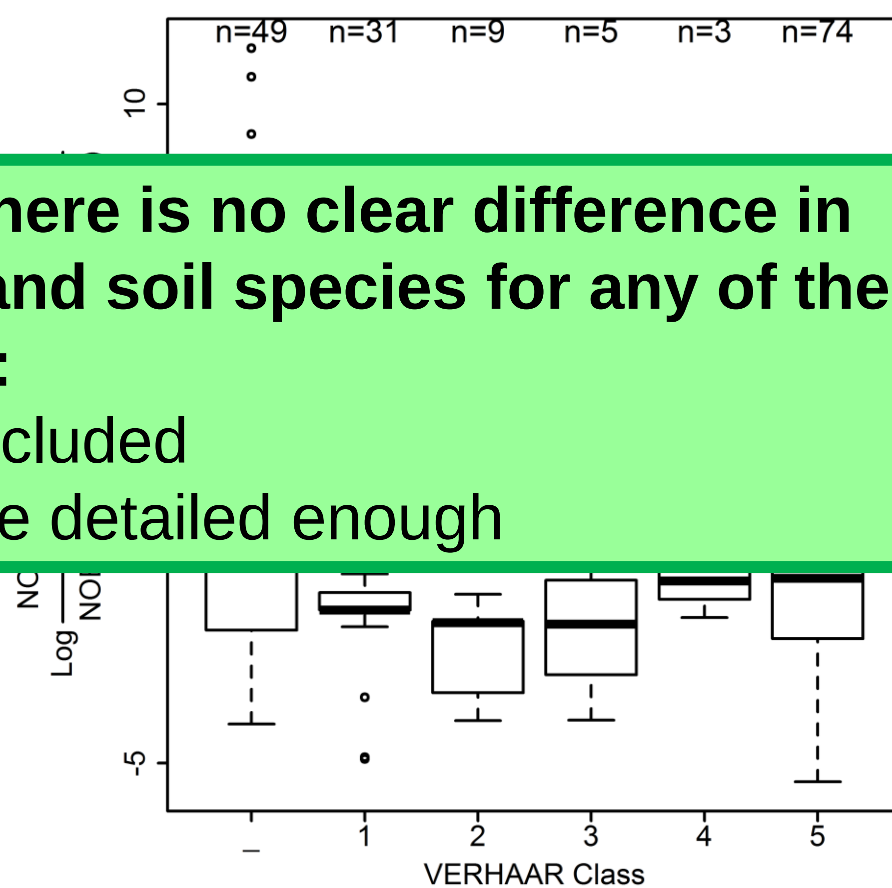
Hazard comparison (II) – Role of phys-chem & MOA

MOA - Versus VERHAAR (aquatic vs soil <u>invertebrates</u>)

Acute



Chronic

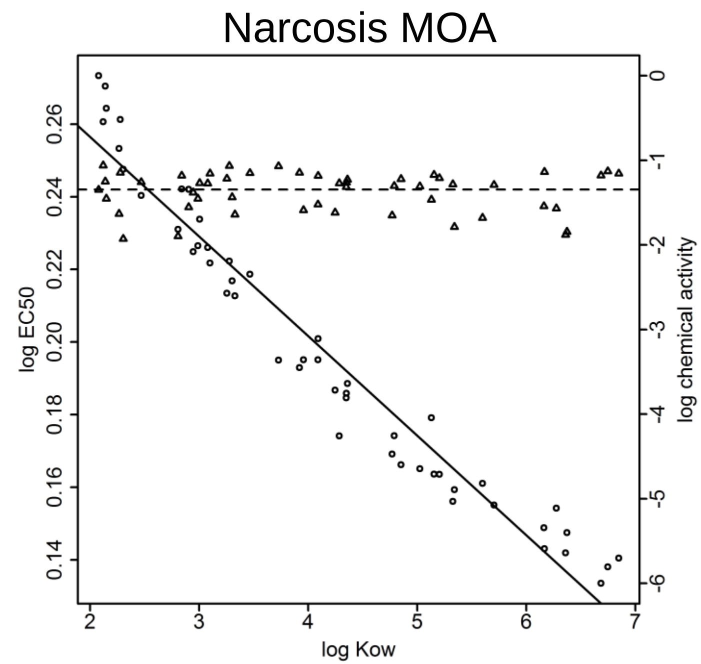


- **Based on VERHAAR class, there is no clear difference in sensitivity between aquatic and soil species for any of the MOAs, but keep in mind that:**
  - Only industrial chemicals included
  - VERHAAR class may not be detailed enough

Hazard comparison (III) – Chemical activity

Chemical activity is the fraction of saturation

$$\gamma = \frac{\text{Concentration}}{\text{Solubility}} \not> 1$$



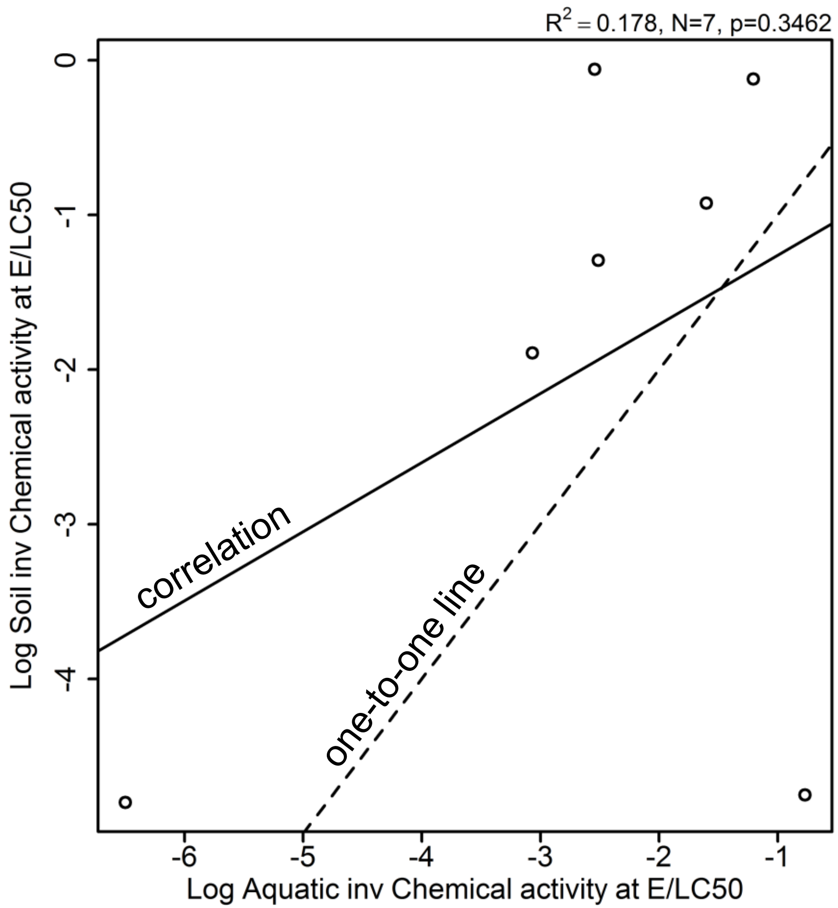
Oversaturation ($\gamma > 1$):

	Acute	**Chronic**
Aquatic	37.5%	52.9%
Soil	84.5%	74.1%

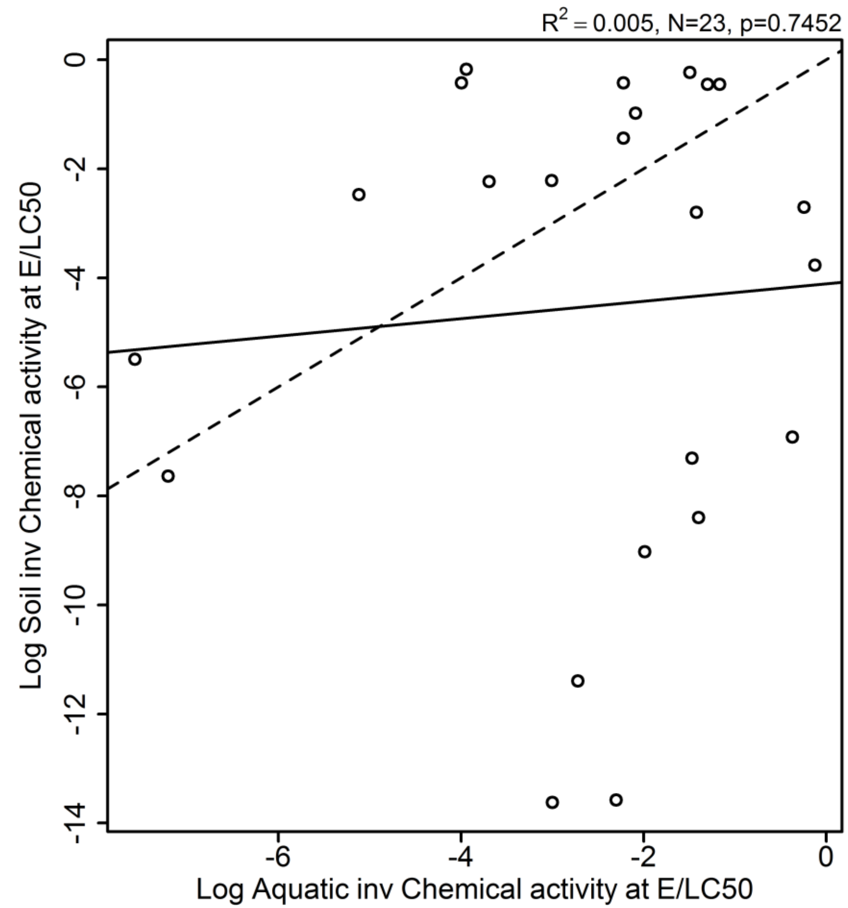
Hazard comparison (III) – Chemical activity

Aquatic vs. Soil invertebrates

Acute



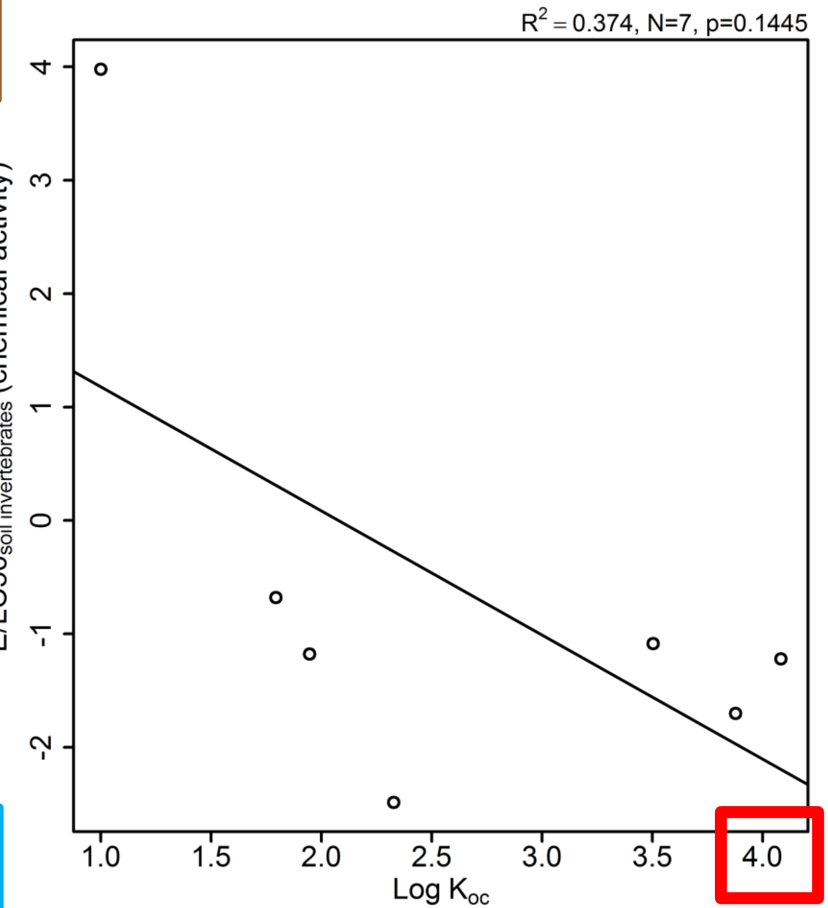
Chronic

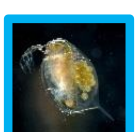


Hazard comparison (III) – Chemical activity

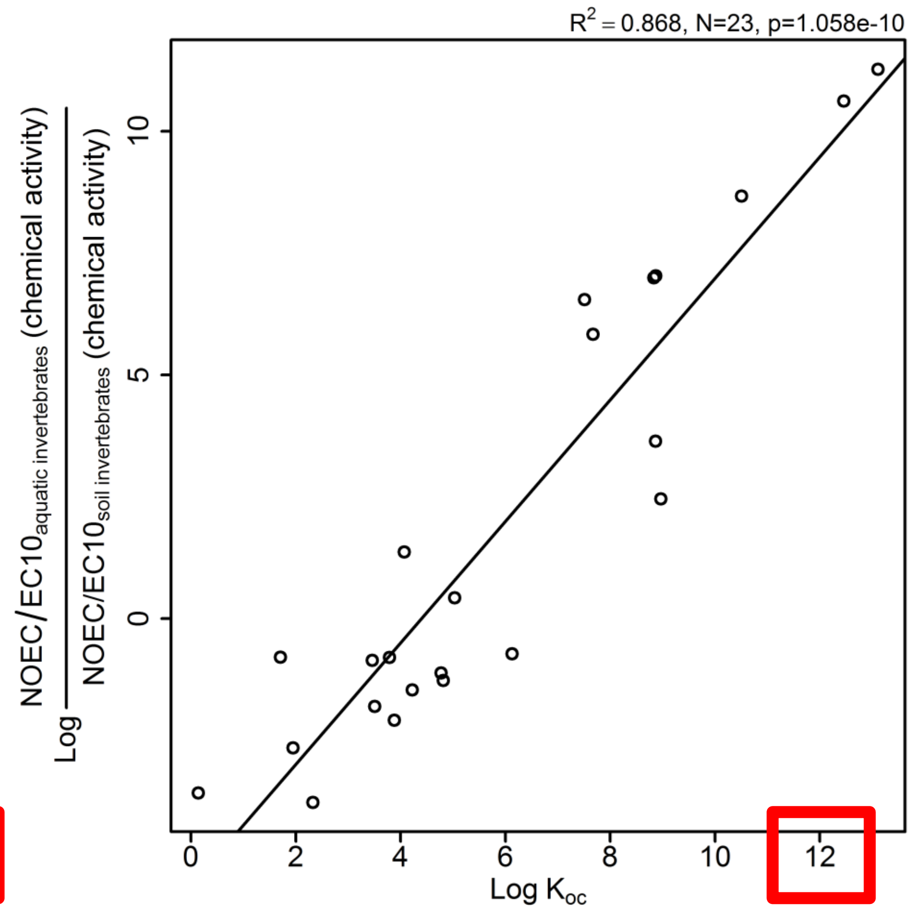
PC – Versus log Koc

Acute





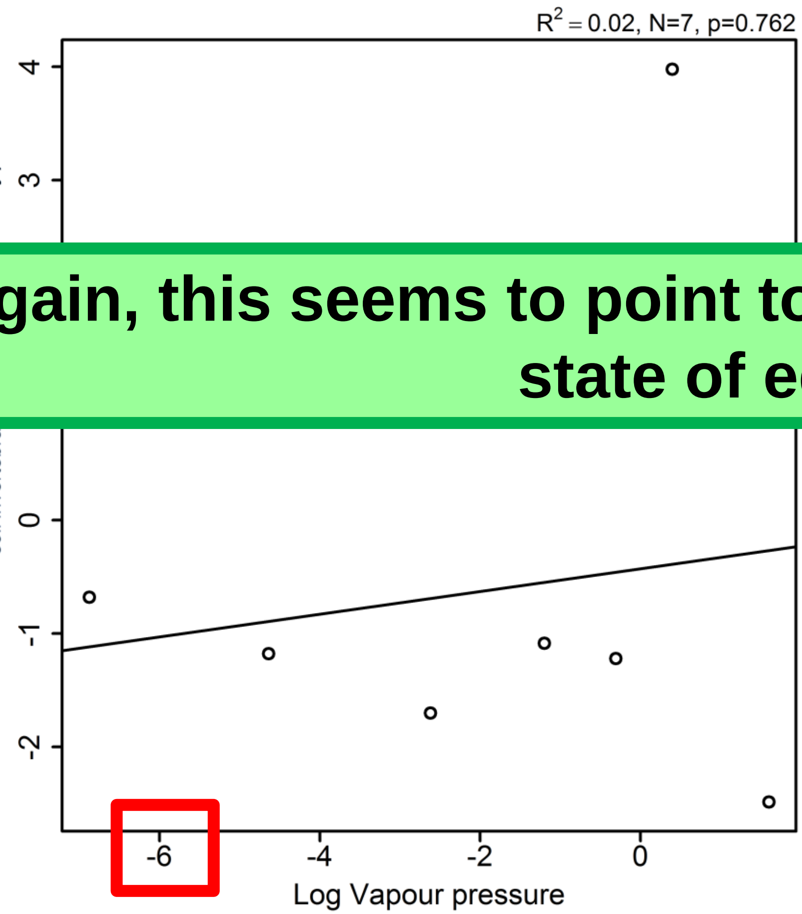
Chronic



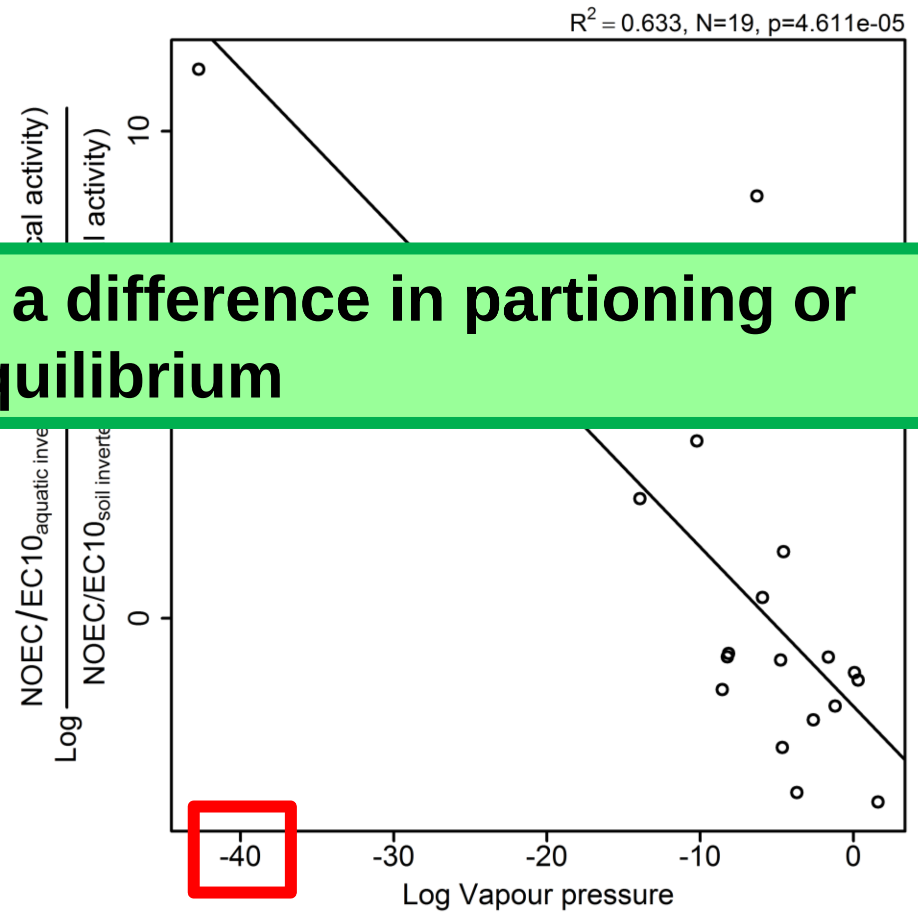
Hazard comparison (III) – Chemical activity

PC – Versus Vapour pressure

Acute



Chronic



Again, this seems to point to a difference in partioning or state of equilibrium

Risk assessment (IV) – PNEC/Risk

REACH **soil** PNEC derivation

Option A

- Experimental soil EC50
- Assessment factor (AF)

$PNEC_{soil,AF}$

Option B

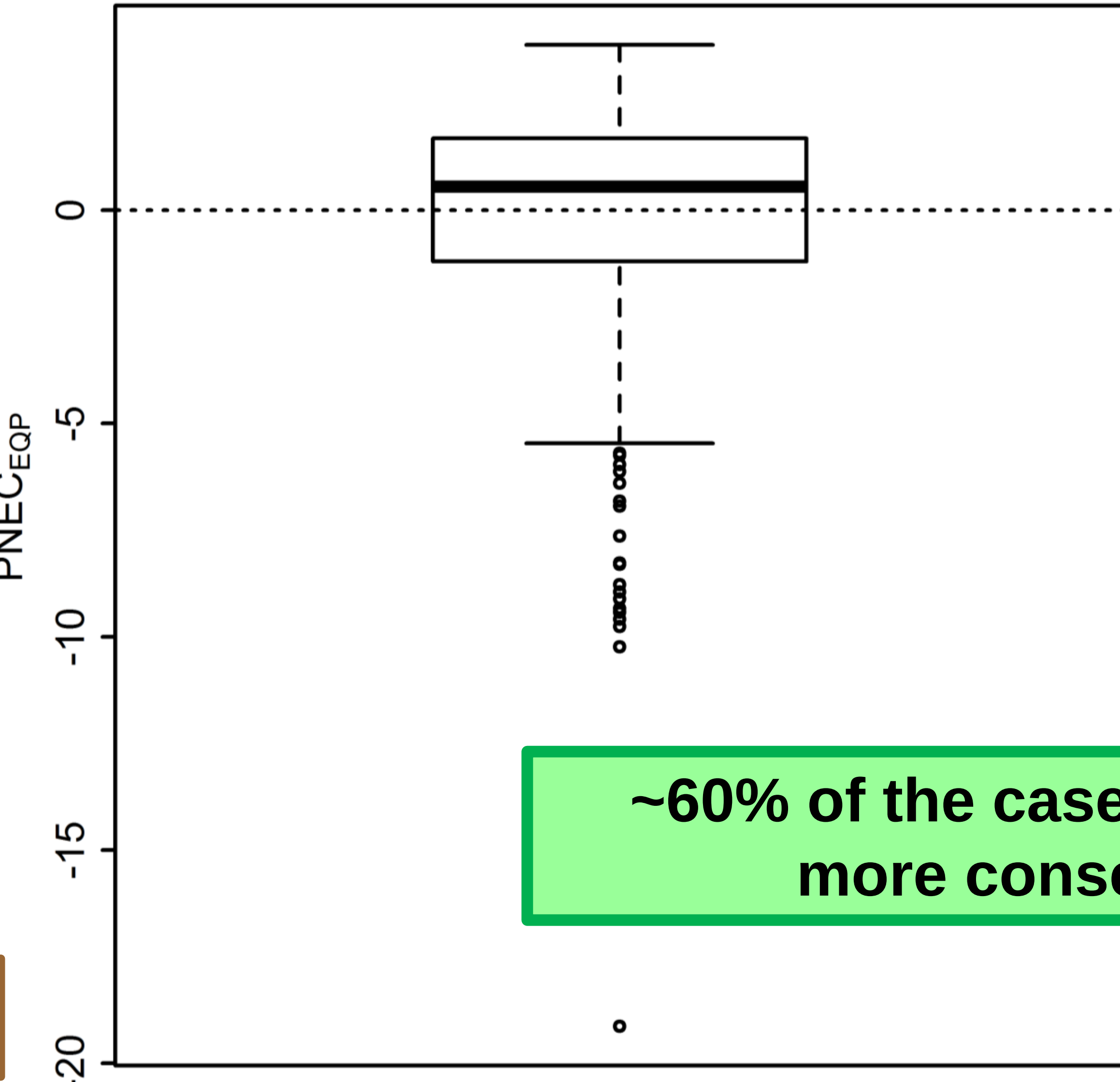
- Experimental aquatic EC50
- Equilibrium partitioning (EqP)

$PNEC_{soil,EqP}$

? =

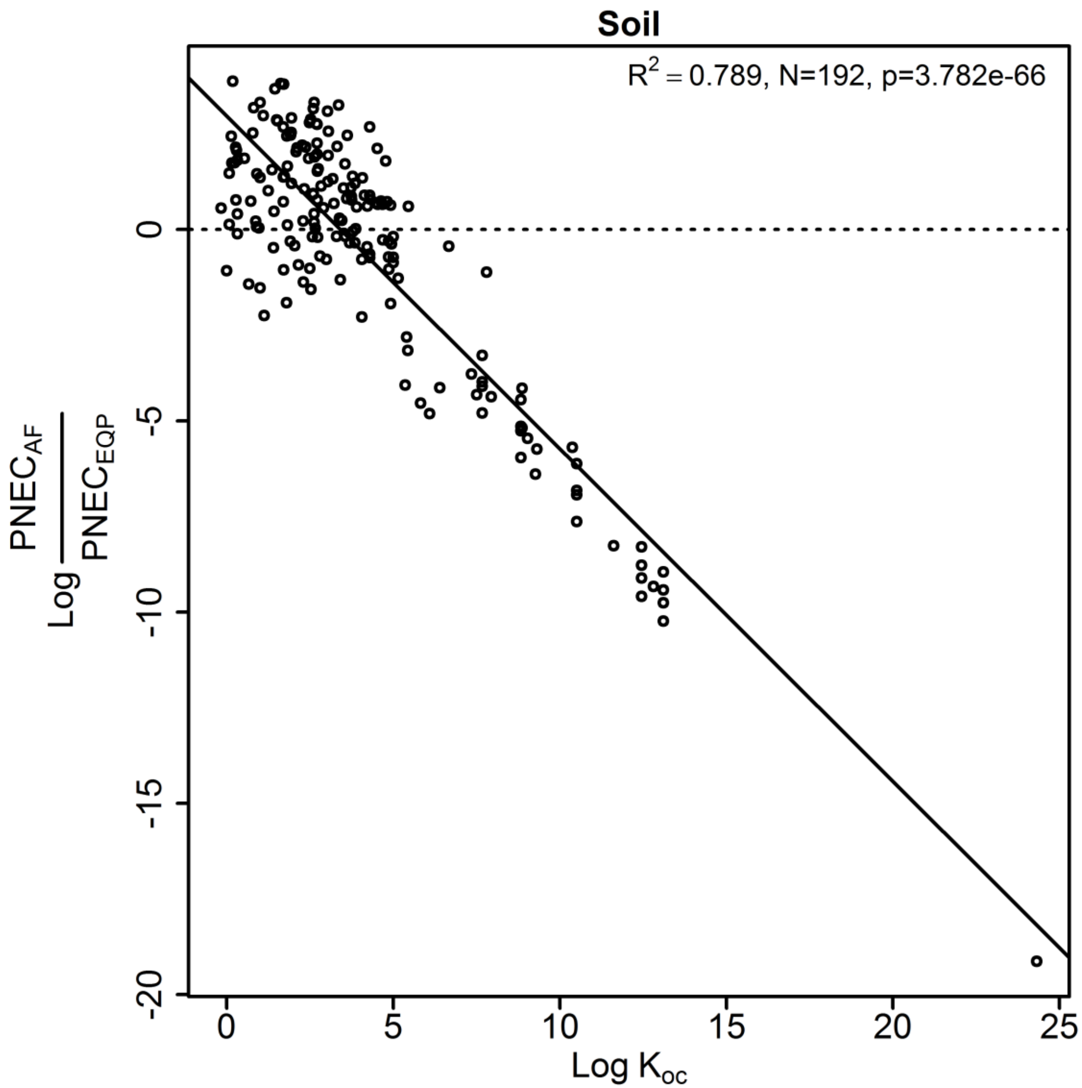
Do we miss any risks when using $PNEC_{soil,EqP}$?

Risk assessment (IV) – PNEC/Risk

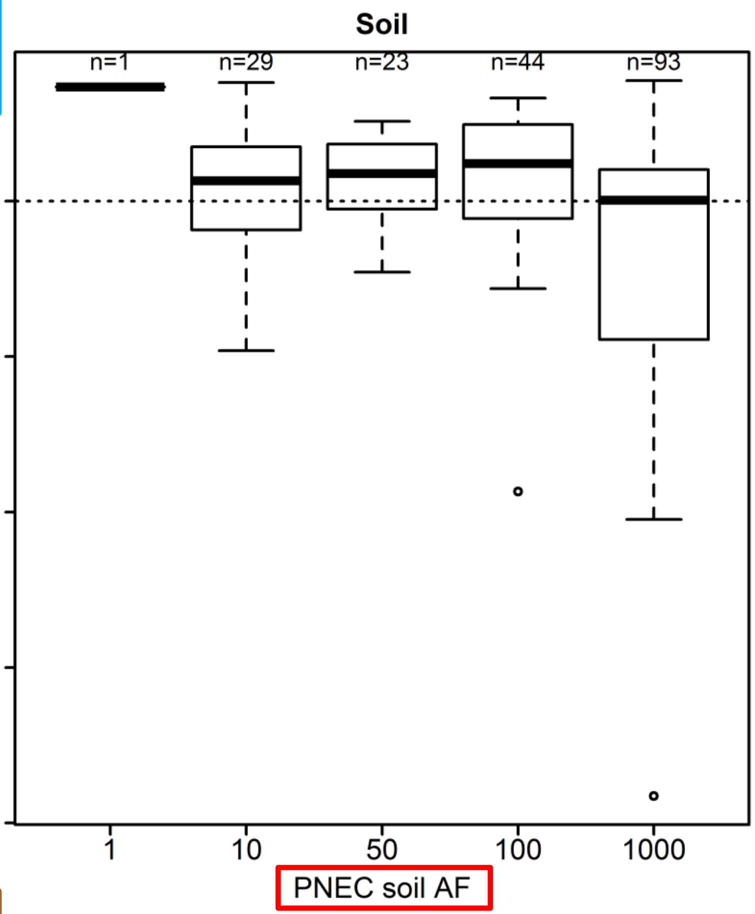


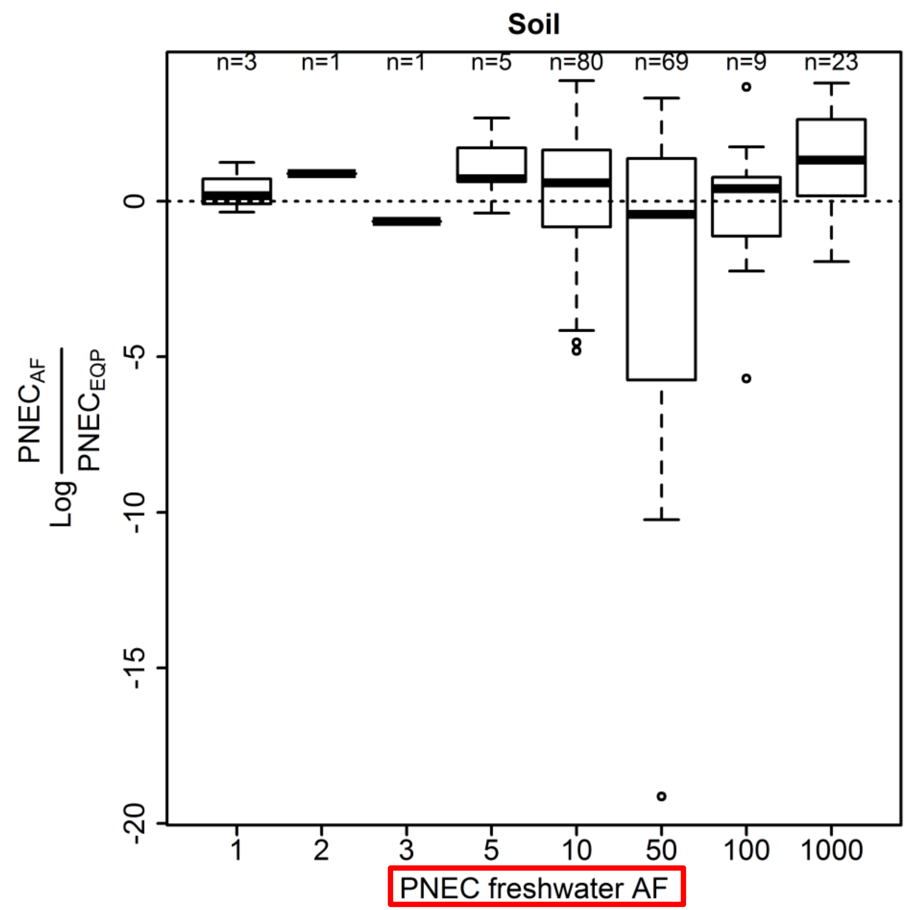
~60% of the cases $PNEC_{EQP}$ is more conservative

Risk assessment (IV) – PNEC/Risk



Risk assessment (IV) – PNEC/Risk





Conclusion & Suggestions

- Role of MOA unclear
- There is a clear link with K_{oc} (and VP?)
  - The hazard to soil invertebrates relative to aquatic invertebrates seems to increase with rising K_{oc} (and declining VP?)
  - This last observation affects soil RAs based only on aquatic data, warranting caution when using EqP on substances with increasing Koc
  - The data suggest that
    - differences in partitioning and/or equilibrium state between aquatic and soil ecotoxicity studies could be the underlying cause
    - The role of contaminant uptake via food is unclear

THANKS

- Stewards and members of the TF

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  Christine Yannakas, Diana Buksa, Ian Cummings

- ECHA

- **For your attention!**