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Welzijn en Sport

Overview of processes driving the exposure of chemicals in soil

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07 October 2015 – Helsinki

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Environmental exposure and fate assessment

1. Elements, processes, parameters driving exposure
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3. Specific aspects
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General

Current Risk Assessment:

Risk = Ratio between exposure (PEC) and effect (PNEC)

Risk = PEC/PNEC (REACH)

Risk = EC_{50}/PEC = TER (PPPs)

PECs are normally based on analyses or modelling of Total Content (TC)

“Soil: the foreseeable concentration of the active substance or any other substance of concern, or of relevant metabolites or breakdown or reaction products in soil” (Presentation Dr. José Tarazona)

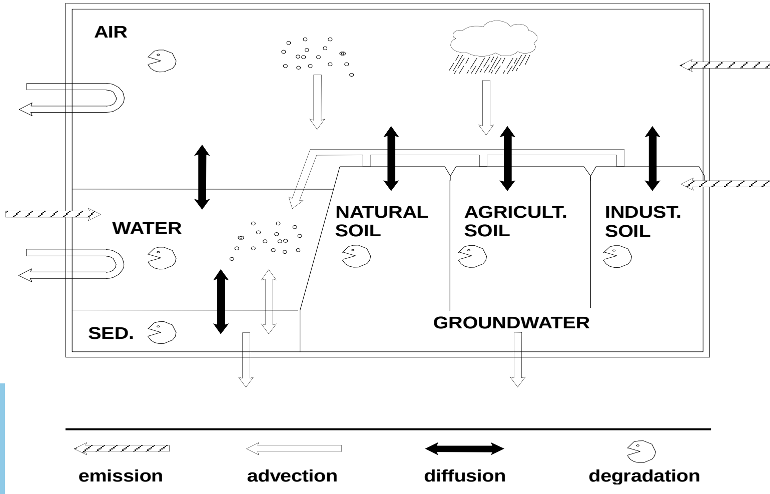
General


M
$K_{Fe\text{-}M}$
M
$K_{Al\text{-}M}$
DOM
AlO_x
K_{OM}
FeO_x
MnO_x
POM
$K_{Mn\text{-}M}$
Clay
M
$K_{POM\text{-}M}$
$K_{Clay\text{-}M}$
M
M

General

- Soil: complex matrix, inhomogeneous, various processes
- Significantly different toxicity at the same total concentration in various soil types
- Numerous studies show reduced toxicity in aged soil
- Effective exposure dependent on: substance specific emission pattern, soil properties, substance properties, timing of emission, weather/climate, ageing, …….
- Simplified approach to PEC
 assessment, too simple?!

➔ Various processes/properties
determine exposure



1. **Elements**, processes, parameters driving exposure

- Compartment specific emissions, application pattern
- Chemical properties of the substance:
  - Partitioning coefficients
  - Degradation kinetics
- Environmental parametrization:
  - Distribution, composition, size of compartments
  - Advective, convective transport fluxes
  - Properties compartment: T, pH, DOC, ….

- Properties may be derived from these key issues: bioavailability, bound residue formation, uptake rates (biota), secondary poisoning ….

1. Elements, processes, parameters driving exposure

- In general: relevant phys.chem. properties and exposure relevant processes well known (common substances)
- Less known: actual bioavailability, actual toxicological interfaces with biota ➔ need to match exposure metrics and chemical forms with metrics used in ecotox. testing

- Also to be considered: impact soil composition/ decomposition/weathering, and climate on fate processes ➔ factor time
- Impact of soil biota on fate: uptake, bioturbation?
- Chemicals with specific interactions (like ionizable substances)
- Key question: relevance of soils used for testing and need to consider non-homogeneous nature of soils

1. Elements, processes, **parameters** driving exposure

General observation: key parameters depend on purpose of assessment. Examples:

- Identify potential for direct physical hazards posed by a chemical or material;
- Determine compartments into which chemical will partition;
- Estimate potential/likelihood bioconcentration, bioavailability and likelihood of toxicity;
- Estimate potential human exposure

1. Elements, processes, **parameters** driving exposure

Substance related key parameters

- Half-lives in soil – biodegradation, hydrolysis, volatility;
- Partitioning coefficients;
- Speciation/nature transformation products;
- Solubility, vapour pressure, BCF, … (dependent on level of detail of assessment)

Soil related key parameters

- Soil type/nature and texture;
- Erosion rate;
- Resuspension rate;
- Horizontal and vertical mass transport (tilling, bioturbation, cryoturbation, leaching, drift, facilitated transport)
- CEC, OC, Clay, pH, redox, T, moisture content, air content

1. Elements, processes, **para-meters** driving exposure

Indirect exposure routes

- Long distance transport + deposition persistent, high volatility substances;
- Sewage sludge;
- Run off

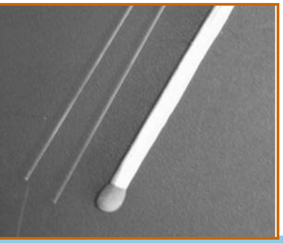
Conditions to take into account

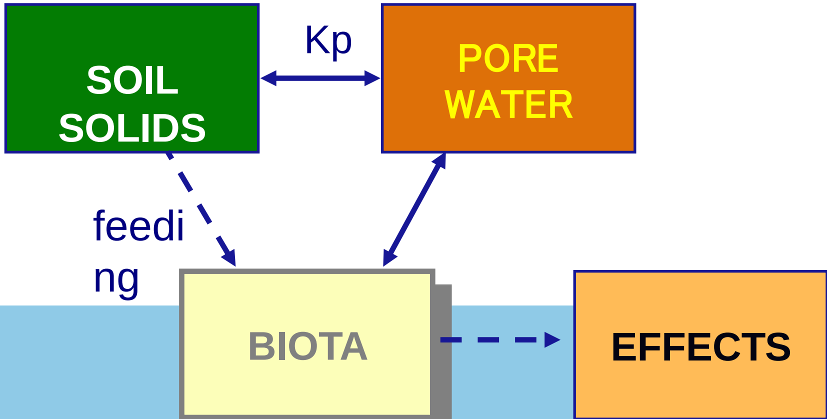
- Poor agricultural practises;
- Change soil pH;
- Precipitation – atmospheric particle content;
- Soil OC content;
- Persistency in general

1. Elements, processes, **para-meters** driving exposure

Improvement of exposure assessment

- Concentrations of chemical in pore water, bound to soil matrix, and soil air concentration might be better metrics of actual exposure;
- Distribution of exposure between pore water pathway and particles ingestion pathway key issue;
- Actually measured instead of nominal concentrations strongly preferred;
- Proper analytical verification as initiated by soil extraction;
- Deploy relatively novel approaches like passive sampling





Modelling

- Extrapolate limited # studies/data to: release scenarios, exposure scenarios, effect scenarios, landscapes)
- EUSES, FOCUS: homogeneous compartments
- Useful to integrate models in tiered RA approaches, but may not fully reflect reality ➔
- Uncertainty in input and model assumptions to be explicitly considered – validation necessary – default parameters require continuous update
- Preferred: assessment long term fate to link to long term effects studies: e.g. landscape-based modelling, GIS mapping, climatic conditions →more accurate PEC

Modelling

- Future: Not necessarily complex modelling tools
- Future potential: handling spatial aspects – geographical info (distribution of key parameters: T, rainfall, soil type, pH, ….) ➔ sophisticated numerical models, including main processes and spatially highly resolved
- Important: assess applicability for regulatory purposes, taking purpose of assessment in account (e.g. local/general conditions)

Tools and tests

- Intermediate scale studies – intact soil cores: soil degradation indigenous microflora
- More sophisticated lab/semi field tests – sieved soil mimicking natural fluctuation (T, water regime), sieved soil fed OC to mimic root exudates, undisturbed columns and irradiation, small scale outdoor degradation studies, lysimeter studies including transfer to deeper soil layers, microcosm and mesocosm studies

- Note: appropriate sampling schedules, sampling techniques, and analytical techniques to be applied

Landscape level approaches

- Landscape level considered highest tier of assessment – spatially distributed modelling
- Not yet taken into account in risk assessment – recent EFSA opinion: modelling approach non-target arthropods
- Landscape level approach requires modelling exposure including in-field and off-field exposure
- Potential issue: availability of suited data (geographic data like maps of soil properties, meteorology), limited practical experience – averaging combining data or samples?
- Geostatistical methods/software, backed by monitoring
- Coverage, implementation dynamic processes in numerical models, availability stakeholders, validation?
- PERSAM, PEARL, PELMO could be used for exp. ass. at landscape level

Degradation/dissipation

- Triggers for higher tier exposure testing?
- Representativity of lab tests ←→ field conditions – most relevant simulation studies?
- How to extrapolate across temperatures, OM, etc.?
- When/how to increase realism by inclusion plants, biota, sewage sludge/manure like in valuating field dissipation studies?
- General: what constitutes justified and acceptable WoE?

Animal testing

- Consensus on key properties identifying key exposure pathway and subsequently allow to confidentially minimize animal testing
- Key issue: either make sure (in)direct exposure unlikely or chemical not available for uptake:
  - Kow/Koc
  - Biodegradation potential – chemical reactivity
  - Volatility
  - Solubility
  - Leaching probability
  - Soil properties affecting speciation: pH, redox, OC
- Apply read across

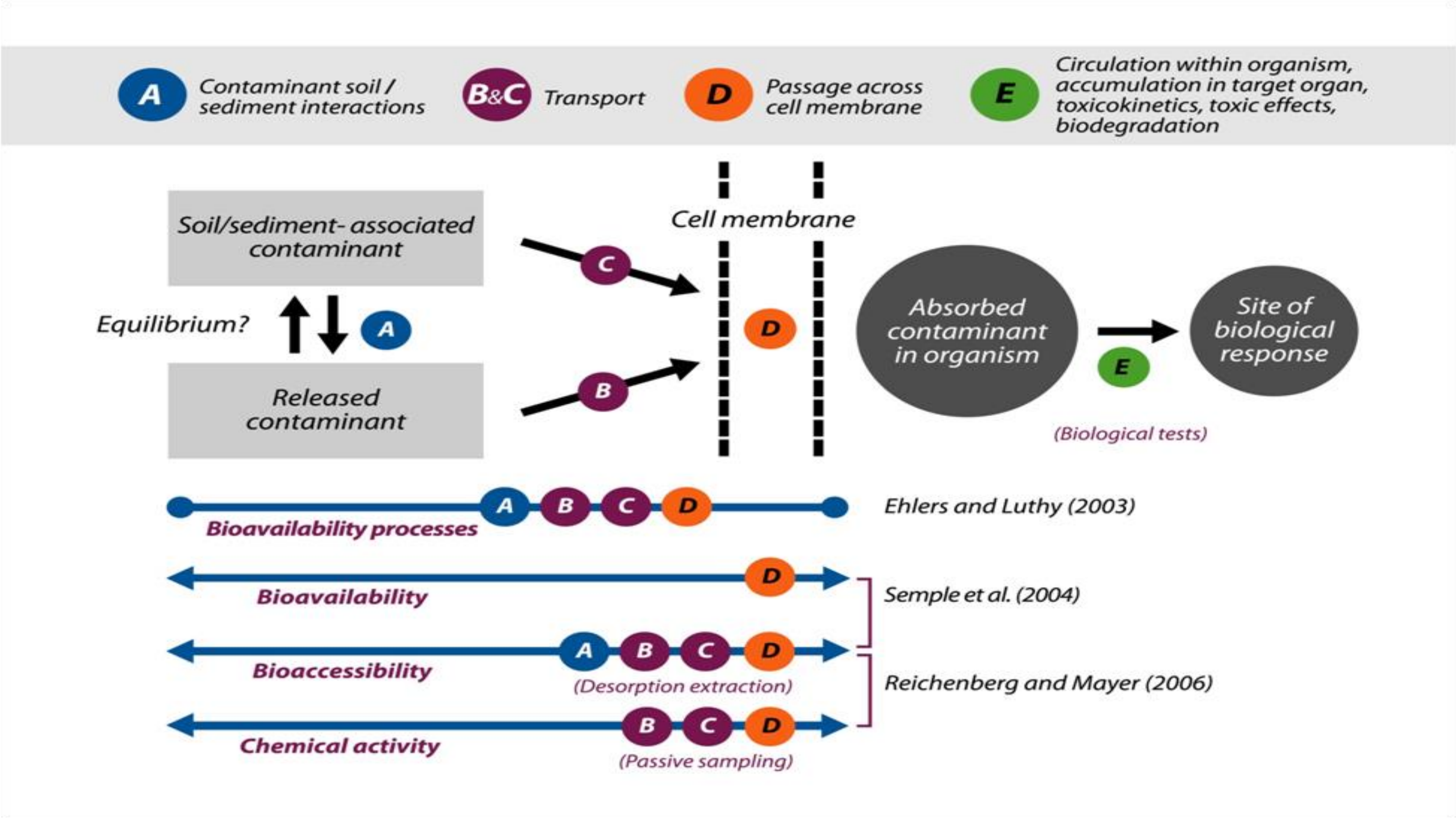
Background concentrations

- To be considered in RA when developing specific protection goals and/or management strategies to reach the goals
- Confusion: natural versus anthropogenic – neither term well-defined ➔ background is scientific/political decision
- Background conc. often not well established, vary at local ←→ EU scale ➔ underestimation of risk possible
- Useful when risks are mapped according to geographical conditions
- Tiered approach – start: highest background concentration, in case unacceptable risk: refine PEC (e.g. use site specific data)
- Added risk approach – take homeostasis into account

Background concentrations - requirements

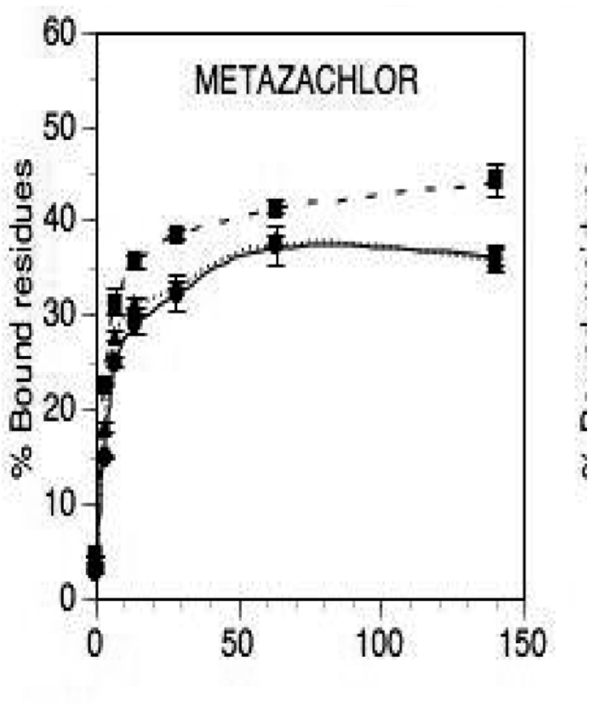
- Sufficient and reliable data: background conc. + bioavailability
- Background concentrations to be presented clearly and as open information
- Total and bioavailable concentrations may differ ➔ “ageing factors” can be used in some cases
- Use of the full application rate applied
- Soil types and regions should be presented
- RA should concentrate on effects of increase of concentrations due to contemporary release of contaminants.
- Account for ability of biota to acclimate to different, environ-mentally relevant, background concentrations
- Soils with low and elevated background concentrations included in fate and effect testing

Bioavailability



Bioavailability/NER

- General premise: adsorption and NER formation reduce availability/effects. However, NER formation not always loss of effect to non-target organisms (exp. route)
- Current RA ignores various NER types – key issue: is residue binding a way of risk reduction?
- Stabilization: assessed case by case basis – appropriate bioassay
- When irreversible binding ➔ assume no effects
- NER assessment: choice of (harsh) extraction method versus modification of chem. structure ➔ introduction of concept of time-dependent sorption (guidance lacking)
- REACH: only degradation not NER formation considered
- Pesticides: NER considered when mineralisation <5% and NER >70%



Metabolite formation - bound residues

Examples non-extractable residues (NER):

- Triticonazole: <10%
- Endosulfan: <12%
- Atrazine: 20-25%
- Chlorothalonil: 5-40%
- Paraquat: >90%

Q:

1. Methodological issues: degree of denaturation of soil in use of extractants
2. Lack of criteria on when "total" extraction is reached – extraction efficiency
3. Ageing – factor time
4. NER = metabolite

Bioavailability

- Correction possible at effects or exposure side
- Metals: empirical bioav. correction justified by mechanistic understanding of processes concerned
- Best metrics depends on target organisms – exposure pathways and exposure conditions
- Q: How to simulate and model bioav./non-bioav. fractions?

Bioaccumulation

- Distinguish bioaccumulation in soil organisms and food-chain (bio)accumulation (or: lower versus higher organisms)
- Models available for assessing bioaccumulation: Kow, Koa, Koc, DT50, pH, %OC, lipid content
- Key: exposure routes – BAF/BSAF hard to predict, allows for more relevant extrapolation of exposure between biota
- Which species to use for testing – only protocol available for earthworms?
- Recommended: include kinetics in assessment: TK/TD
- Internal conc. may be better option than exposure conc. for exposure based waiving
- Metals: regulation and hyper-accumulation to be considered

Summary

- Tiered approach to exposure assessment
- Triggers needed
- Modelling
- Geographical scales: local – landscape levels
- Key differences between REACH and pesticides/biocides regulation
- Increased realism versus simplicity of modelling - complex versus generic modelling and data requirements

Breakout sessions

Topic 2 – group a

1. What are the key elements and processes to be considered in the environmental exposure and fate assessment?
   a. key physico-chemical parameters to be considered in soil exposure and fate assessment
   b. release, transfer/partitioning, aging of the different type of substances; metals, ionisable substances, surfactants
   c. Which processing steps/operational conditions/set of physico-chemical properties would indicate high potential for indirect exposure (e.g. deposition from air or via sludge from WWTPs etc.) of the soil?
   d. What are the key aspects to be taken into account in degradation/dissipation assessment e.g. triggers for testing degradation in soil (simulation testing), relevant temperature for assessing degradation rate, information relevant for Weight of Evidence (WoE)?
   e. What are the key aspects to be taken into account in soil bioaccumulation assessment in regulatory decision making (e.g. bioavailability, test environment, reliability and relevance)?

Breakout sessions

Topic 2 – group a

2. How to take bioavailability and NER formation into account in soil exposure and fate assessment?
   a. How to take into account the bioavailability in soil in relation to effects assessment?
   b. Whether and how NERs should be considered in soil exposure/risk assessment?
   c. Does stabilisation of a substance (NER) always mean a loss of effects on non-target organisms?
   d. How is the formation of bound residues currently taken into account within the different regulations as part of the soil risk assessment (trigger values for further characterisation of the non-extractable residues (NER) and field studies)?
   e. How to reliably identify and quantify NERs within degradation simulation testing in soil?

Breakout sessions

Topic 2 – group a

3. How are exposure and effect assessments linked today? How could they be better linked in the future?

4. Measuring of exposure in ecotox media/studies?

    a. What analytical tools are available at the moment, what are their limitations, and how to improve exposure assessment in ecotox media/studies?

    b. What is the feasibility of testing of exposure concentrations also of metabolites in the standard soil tox/fate strategies?

Breakout sessions

Topic 2 – group b

1. Modelling tools in soil exposure assessment

    a. How are modelling tools used within different regulations today?

    b. What would be the available tools and tests to be used as intermediate tiers from lab to field in the exposure assessment?

    c. Which type of chemicals would require specific soil exposure assessment i.e. modelling tools available for neutral organic chemicals would not be applicable or would need to be adapted? Triggers for specific attention?

    d. Potential of the methods and modelling tools in the future?

    e. What are the possibilities for use of modelling tools for regulatory purposes?

Breakout sessions

Topic 2 – group b

2. How are exposure- and effect assessments linked today? How could they be better linked in the future?

3. What methodology and tools are available today to carry out exposure assessments at landscape level? What data and tools are needed to make it possible in the future?

4. Background concentrations
   a. How might the background concentrations (i.e., natural and/or anthropogenic 'ambient' levels) of soil contaminants be incorporated into the risk assessment process?
   b. How to take into account the background concentrations in risk assessment (PEC)?