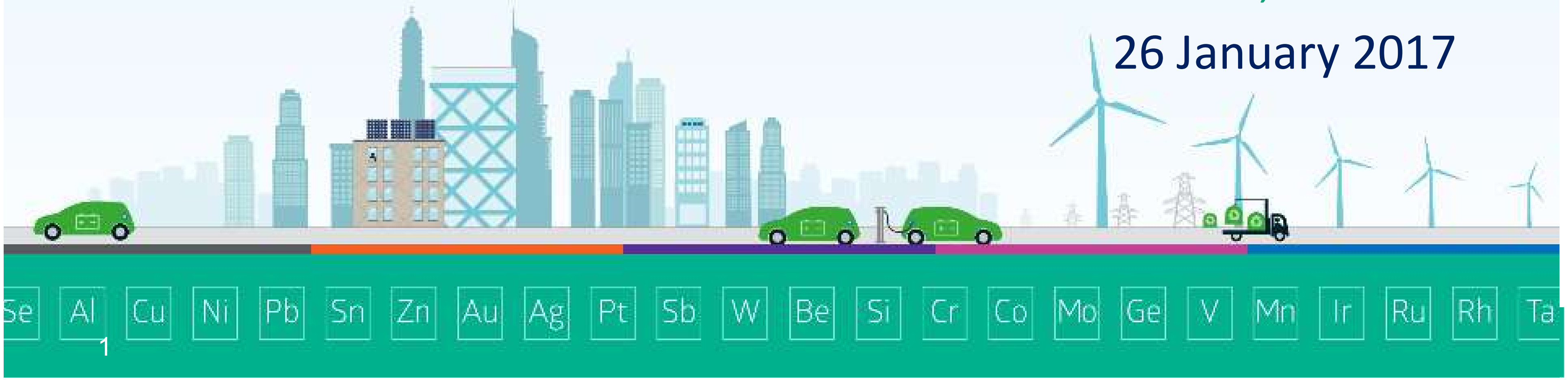
Eurometaux
European Association of Metals

Scientific seminar

Improving the Man via the Environmental Scenario for inorganics with emphasis on metals

Metals Conference Centre, Brussels

26 January 2017



1. Welcome and introduction

Agenda

Welcome and introduction (10h-10h15)

- Agenda
- Seminar organisation, rules and expected outcome and output

1. Scene setting (10h15 – 11h05)

- Different uses of the MvE scenario under REACH, relevance of the MvE scenario to demonstrate safe use and to conduct socio economic assessment, need for generic improvements (Hugo Waeterschoot, Eurometaux)
- How are MvE scenarios built, what are the boundaries of the present model and what refinement needs are already identified? (Joost Bakker, RIVM)

2. Existing experience: from pure modelling with EUSES to refined and monitoring based assessments (11h05-12h50)

- The REACH guidance on MvE in short and a re-cap on the chromates, arsenic MvE modeling in existing AfA cases (Peter Simpson, ECHA)
- MvE scenarios in REACH registration files for metals, Cd case (Frank Van Assche, IZA/Eurometaux)
- A site specific risk assessment on the impact of nickel and chromate compounds on the population surrounding a stainless steel smelter/recycler (Katleen De Brouwere, VITO)

Agenda (2)

3. Modelling aspects and key data sets that may improve the MvE assessment in a tiered way (13h30-15h15)

- What key assumptions drive the technical assessment and can be improved through local/regional data gathering and the sensitivity assessment of key contributing parameters? (Violaine Verougstraete and Hugo Waeterschoot, Eurometaux)
- Modeling ambient air concentration of metals at the local scale: tiered approaches and data requirements, (Wouter Lefebvre, VITO)
- The role and relevance of diet study information in improving the human MvE exposure modeling (Erik Smolders, KUL)
- Alternative modeling options for integrated MvE exposure at the regional and local scale: development of a tiered approach for metals in the MERLIN-expo tool? (Frederik Verdonck, ARCHE and Katleen De Brouwere, VITO)

4. Discussion and way forward (15h25-16h25)

- What are the main data gaps to improve scientifically, for metals and inorganics?
- What are the most relevant tiered data levels to improve the MvE assessment of metals?
- What tiered modelling features could be improved and is MERLIN-expo a good tool for assessing MvE for metals?

Conclusions

Seminar
Organisation, rules, expected outcome and output

Se Al Cu Ni Pb Sn Zn Au Ag Pt Sb W Be Si Cr Co Mo Ge V Mn Ir Ru Rh Ta

MvE Seminar

Objectives:
- Scientific seminar
- Define areas and tiered ways to improve the MvE assesments for metals and inorganics under REACH

Organisation
- Initiative co-hosted/supported by ECHA, RIVM (Nl) and Eurometaux

Rules:
- Exclusively scientific discussion
- Feel free to speak/react as an expert (organisation does not count)
- Chatham house rules

MvE Seminar

Expected outcome:

- Better understanding why EUSES MvE scheme is a “first tier” assessment
- Recommendations on type of data sets that can improve
- Suggested data Tiers to refine the MvE assessment
- Suggested improvements to models to increase relevance for metals and inorganics

Output:

- Meeting report with recommendations (not a summary of the slides)
- Path forward for metals guidance
- Reporting to SEAC/RAC

1. Setting the scene on Man via the Environment

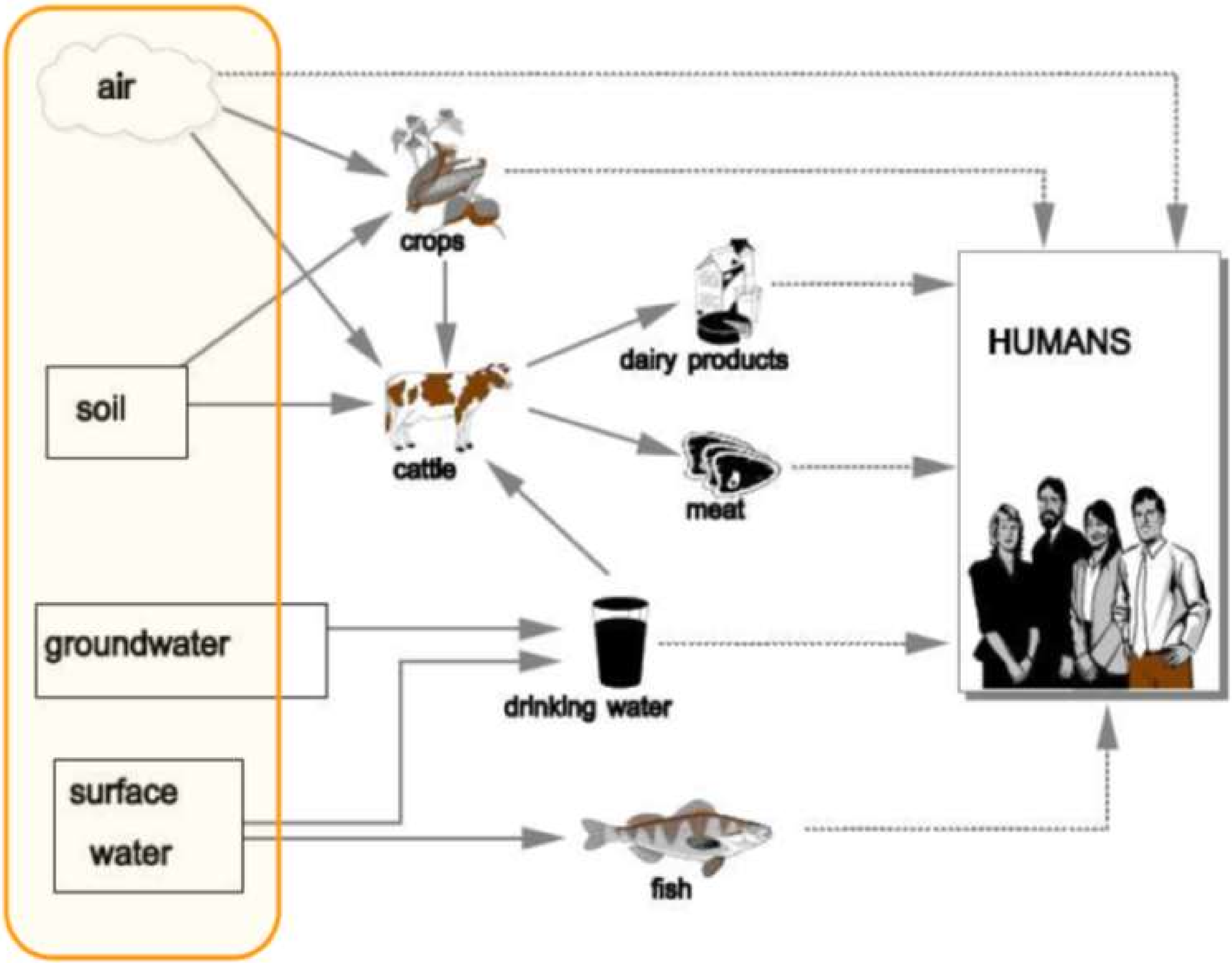
MvE and REACH, relevance of the MvE scenario and need for refinement

By Hugo Waeterschoot,

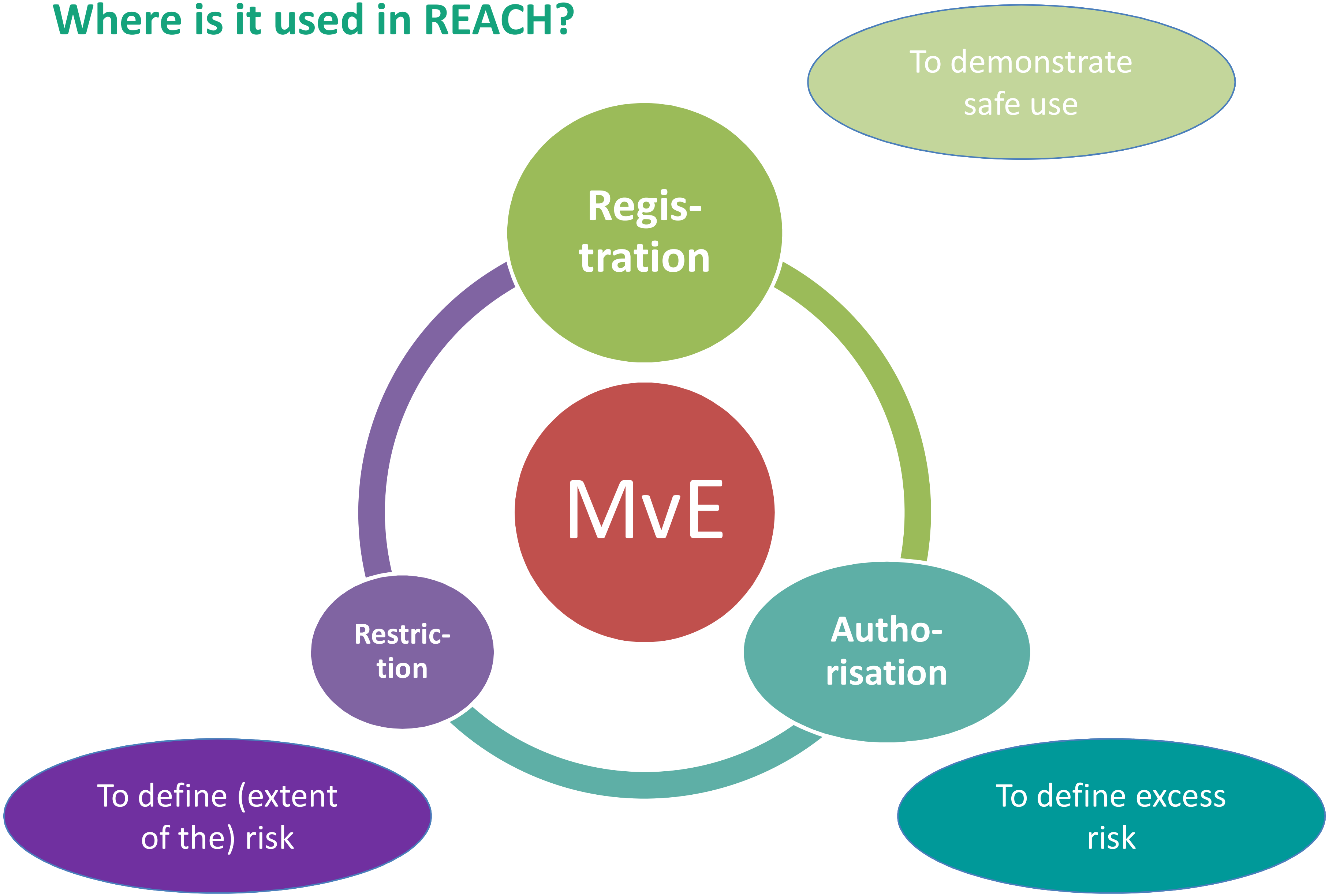
(Eurometaux)

with input from ECHA

The MvE Scenario
Indirect exposure / intake of humans via the environment

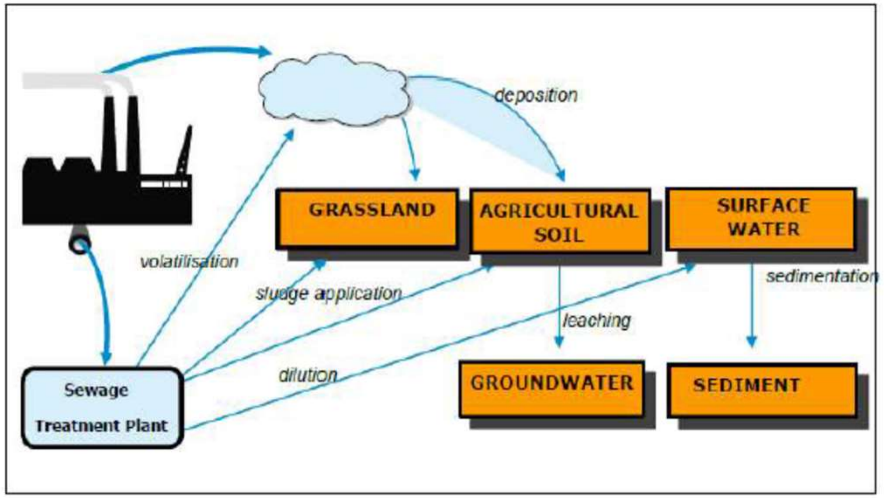


Where is it used in REACH?



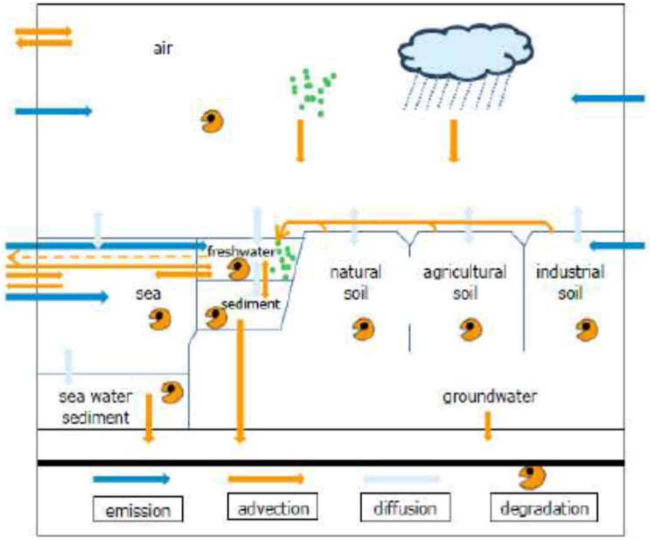
Use for REGISTRATION purposes

Local assessment



Exposure around release point

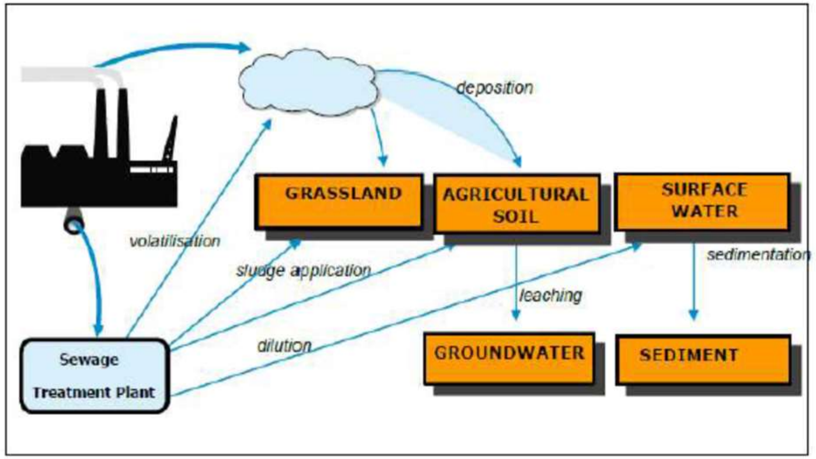
Regional assessment



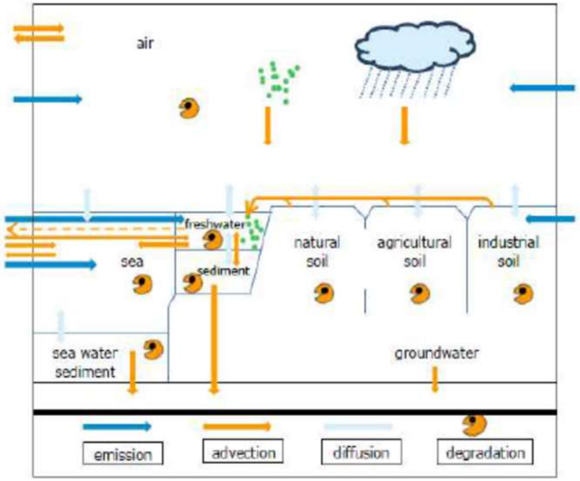
Integrated exposure background (point and diffuse sources)

How does it work (2) ? *A Local & Regional Dimension*
First step: Exposure and fate

Local assessment



Regional assessment



Modelled

Exposure around release point

Simple fate model

All food and water from **local area**

All release from a **single source**

Minimal dilution

Standard surroundings 10000 inhabitants

Integrated exposure background

Multi media fate model

Steady state assumption

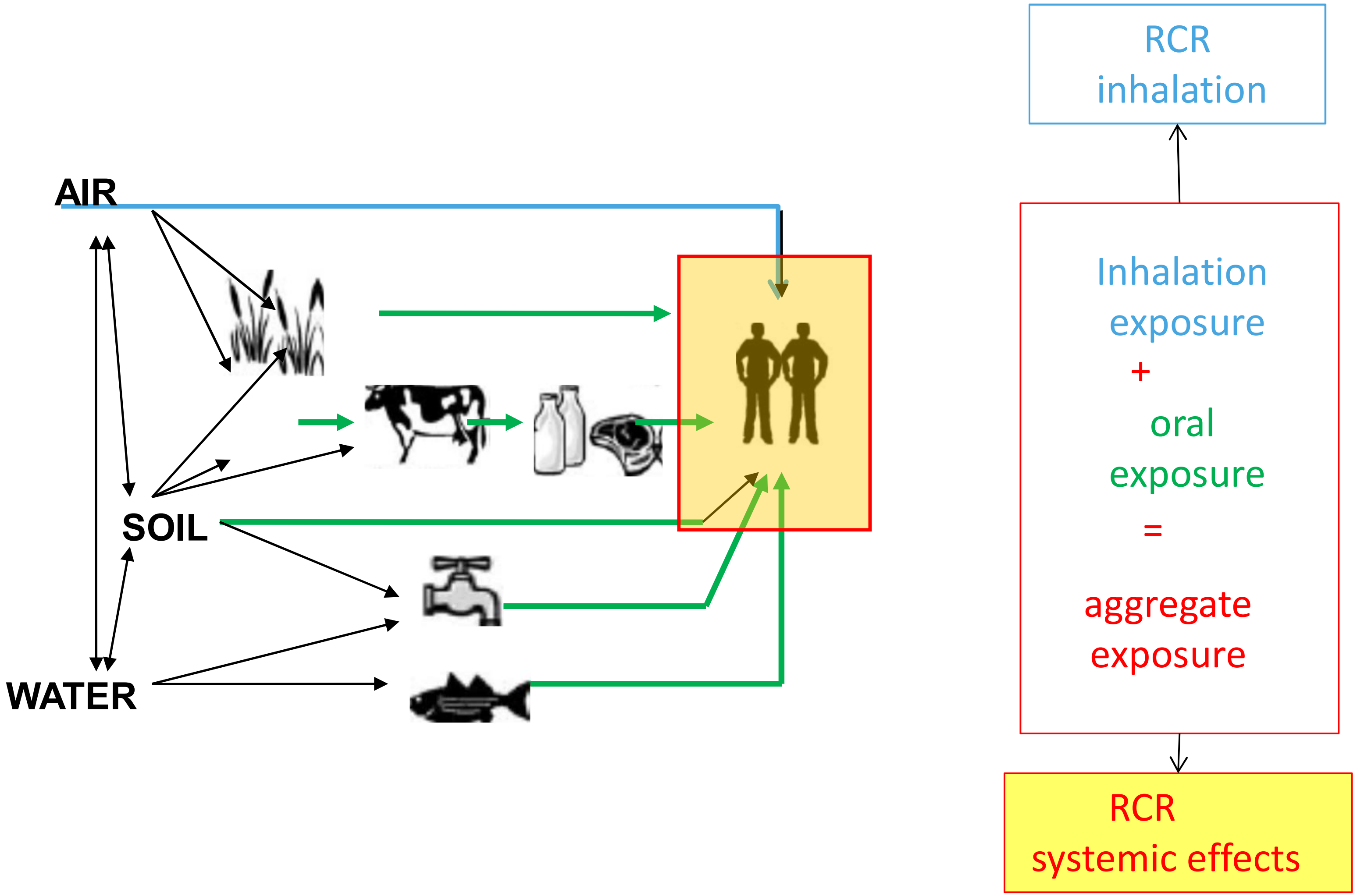
All sources used

WWTP sludge used

10 % of EU size, 20 mio inh

Or monitoring data

How does it work?
Second step: intake and effect estimation



Used for AUTHORISATION applications
To estimate "excess risk"

Example of Man via the Environment assessment in a recent AfA case on Chromium trioxide use for Functional Chrome Plating

Estimated additional statistical fatal cancer cases, based on 40/70 years of exposures, RP applied for, 1 year of exposure)

	Exposure duration per day (h)	Exposure 8h adjusted TWA (µg/m³)	Excess lung cancer risk	Number of exposed people	Estimated statistical fatal cancer cases (years of exposure)		
					40 y	12 y	1y
Workers – Combination of WCS	<1	0.25	0.001	4392	4.39	1.32	0.10
	1-3	0.75	0.003	2062	6.19	1.86	0.16
	4-6	1.5	0.006	2289	13.73	4.12	0.34
	6-8	2	0.008	7608	60.86	18.26	1.52
	Not regularly exposed	0.25	0.001	6577	6.58	1.97	0.16
Workers total				22928	**91.75**	**27.53**	**2.29**
	Exposure 24h (µg/m³)				**70 y**	**12 y**	**1 y**
Man via environment - Local	2.85×10^{-6}		8.27×10^{-5}	10,000 x 1,590 sites = 15,900,000	**1314.93**	**225.42**	**18.78**
Man via environment - Regional	Not relevant						
Total					1406.68	252.94	21.08

Man via the Environment scenario is often it an issue for Risk Management?

Often the weakest link in the RMM assessment for Restriction and Applications for Authorisation

Due to ***concept*** and ***methodological aspects*** and ***lack of case specific data***

The need to do a *Man via the Environmental Assessment*?

"*The need for*" is clear from the REACH Legal text as from the SEA AfA guidance:

REACH legal text (Annex I)

> *"An estimation of the **exposure levels** shall be performed for **all human populations** (workers, consumers and humans liable to exposure indirectly via the environment) [...] for which exposure to the substance is known or reasonable foreseeable".*

Section 5.2.4 (Exposure assessment)

> *"The **risk characterisation** shall consider the human populations (exposure as workers, consumers or indirectly via the environment and if relevant a combination thereof) [...] for which exposure of the substance is **known or reasonably foreseeable**".*

Section 6.2 (Risk characterisat

ECHA SEA guidance

> *Human health impacts may follow from:*
> - *Exposure of workers*
> - *Exposure of consumers*
> - *Exposure of **man via the environment** (e.g. via inhalation of ambient air and consumption of contaminated food and drinking water)*

Section 3.4.3.1 - Background

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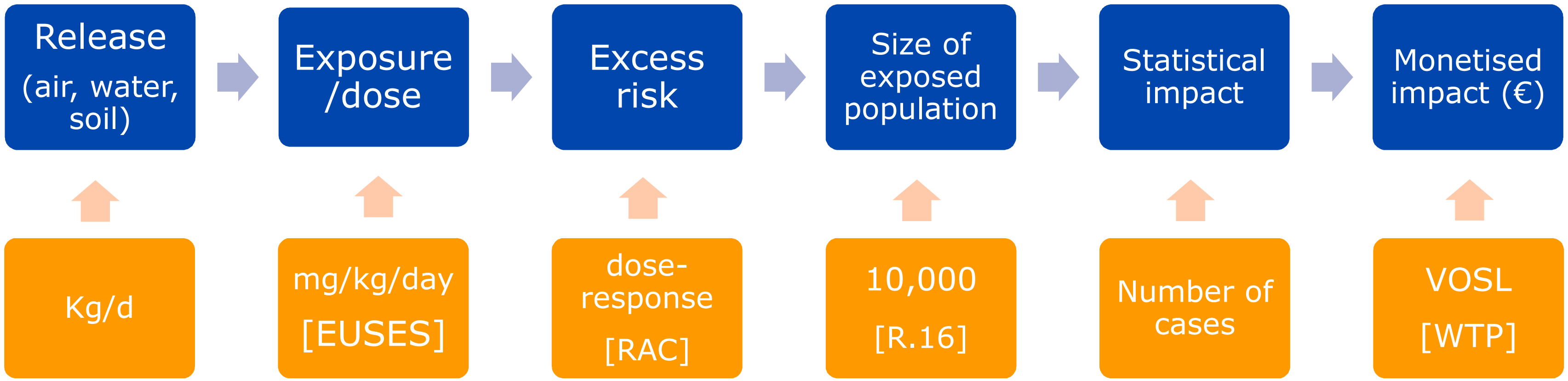
Impact in the general population

- Impact can be simply estimated as:
  - Exposure x dose-response x population size = statistical cases
  - Monetised impact = statistical cases x reference value (WTP*)



*Willingness To Pay

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

1. Setting the scene on Man via the Environment

EUSES scenarios for man exposed via the environment

By Joost Bakker,
(RIVM)

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

Contents

1. EUSES background
2. Local exposure
3. Man via the environment

EUSES background

- Purpose of EUSES
  - Original developed for quantitative hazard and risk assessment of new and existing chemicals in 1993
  - harmonised, general scheme for rapid assessment at the initial and intermediate level, for neutral organic compounds
  - Screening purposes, often worst-case assumptions
  - To identify critical exposure routes
  - Need for refinement (emission, distribution, exposure)

- Limitations
  - Not intended to be used for site specific assessment
  - process formulations are sometimes based on limited research and need to be improved such as transfer from soil and feed to cattle, transfer to drinking water

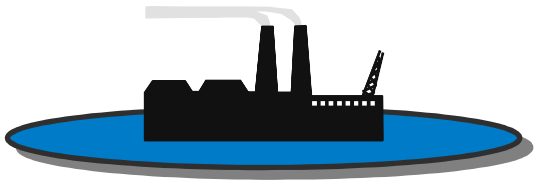
EUSES background

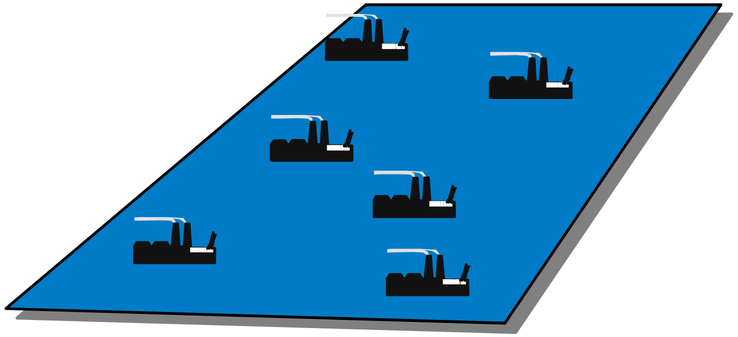
- Latest update (2004)

- EUSES integrated in CHESAR for Chemical Safety Assessment under REACH mainly for the
  - Environmental distribution module
  - Exposure module

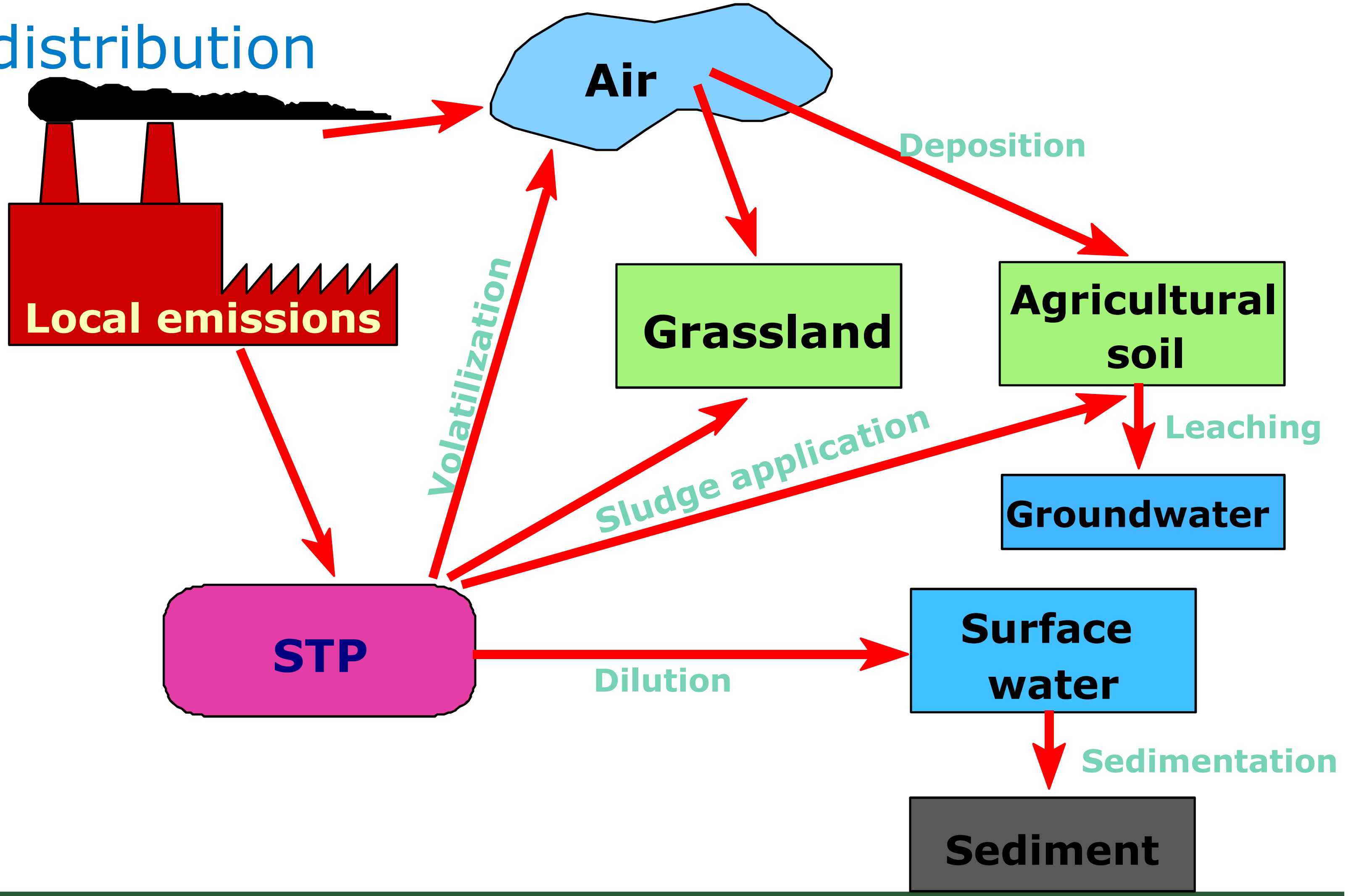
Indirect human exposure assessed for two spatial scales:

- Local scale
  - Around a point source
  - Sewage treatment plant
  - 100% consumption from area around point source
- Regional scale
  - Larger area (country)
  - case: 200 x 200 km with 20 million inhabitants
  - 100% consumption from region





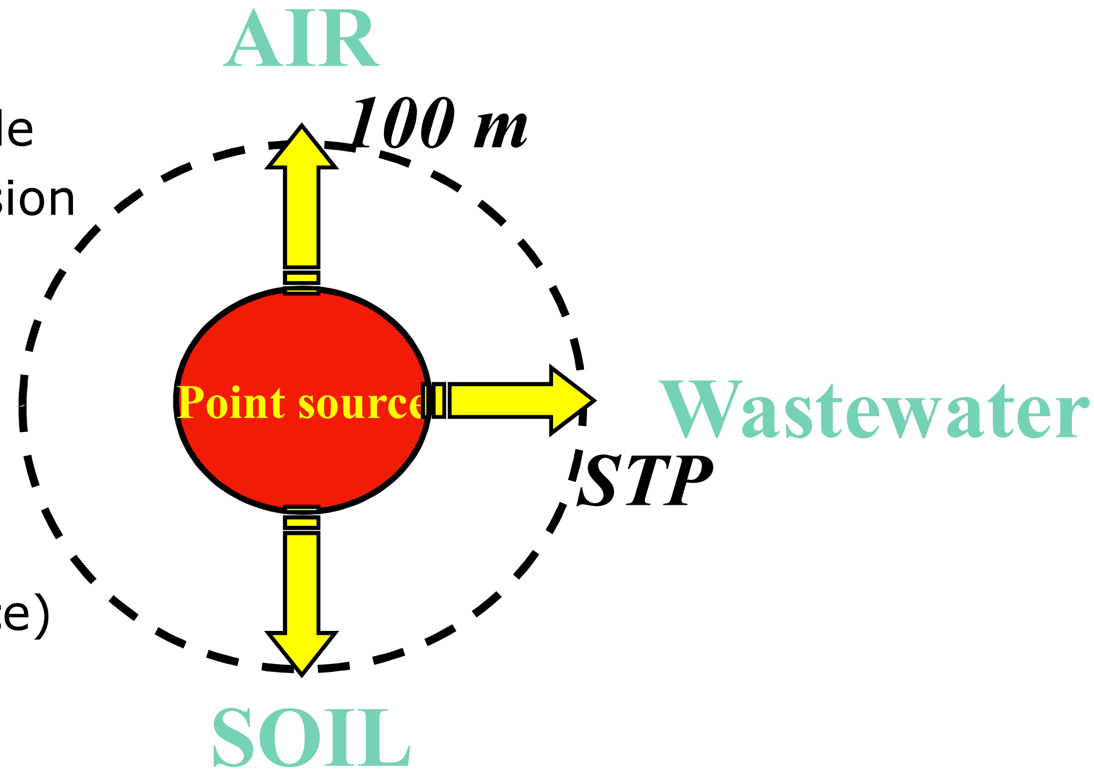
Local distribution



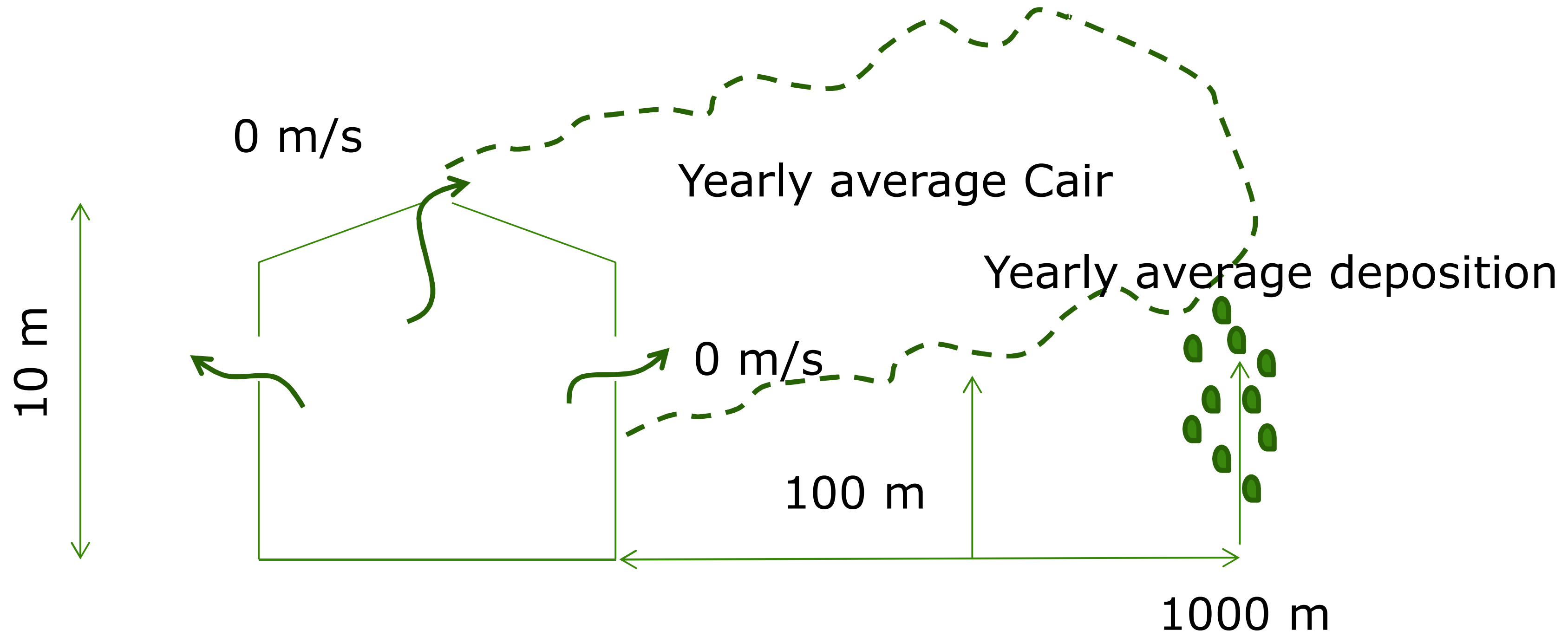
Local Exposure models

- Sewage treatment plant
  - Simpletreat version 3.0
  - Capacity 10,000 inh. eq.
  - One STP for each life cycle stage, no aggregated emission

- Local air concentration, source characteristics:
  - Height 10m
  - No heat content
  - No size (ideal point source)



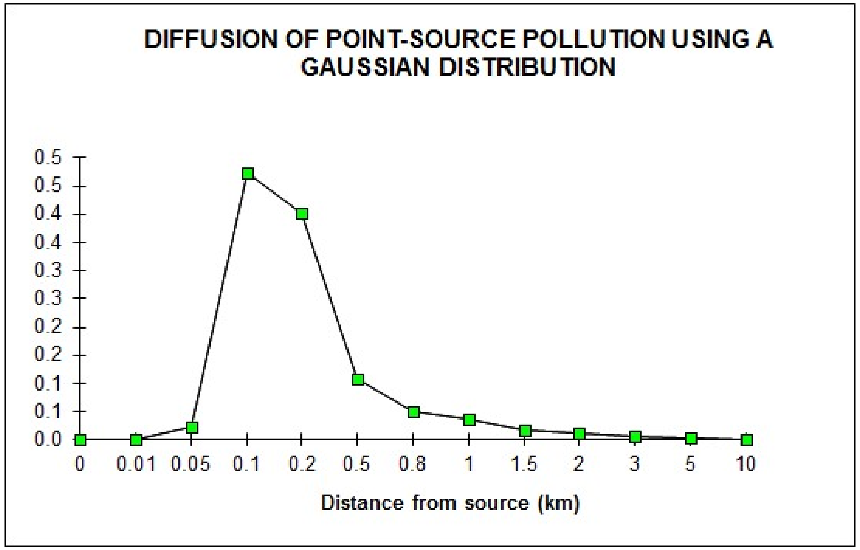
Local model for air concentration

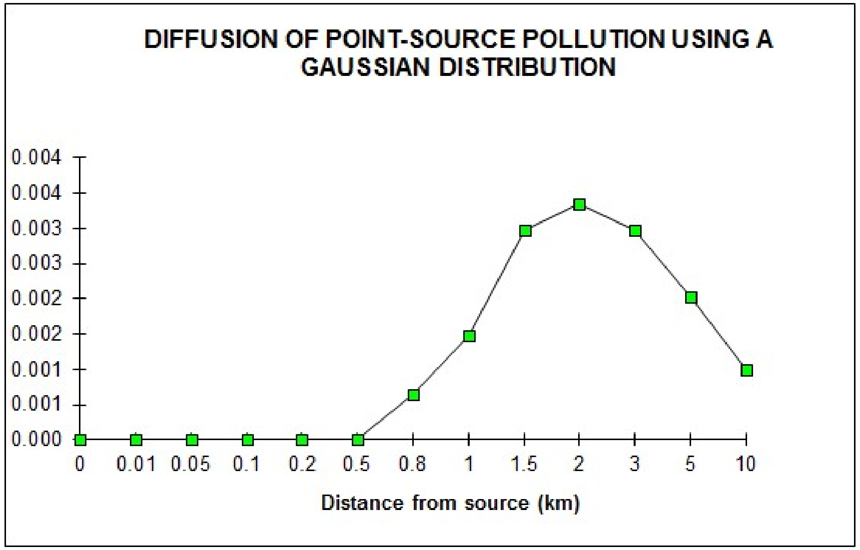


Local air distribution model

- Physical mixing processes are dominant at short distance
- Therefore simple linear relationship between source strenght and concentration can be assumed
- The constant is calculated with the Gaussian plume model OPS
- $Clocal_{air} = \max\left(Elocal_{air}, Estp_{air}\right) \cdot Cstd_{air}$
- Dep = (Elocal + Estp) * $Cstd_{dep}$

Effect source characteristics

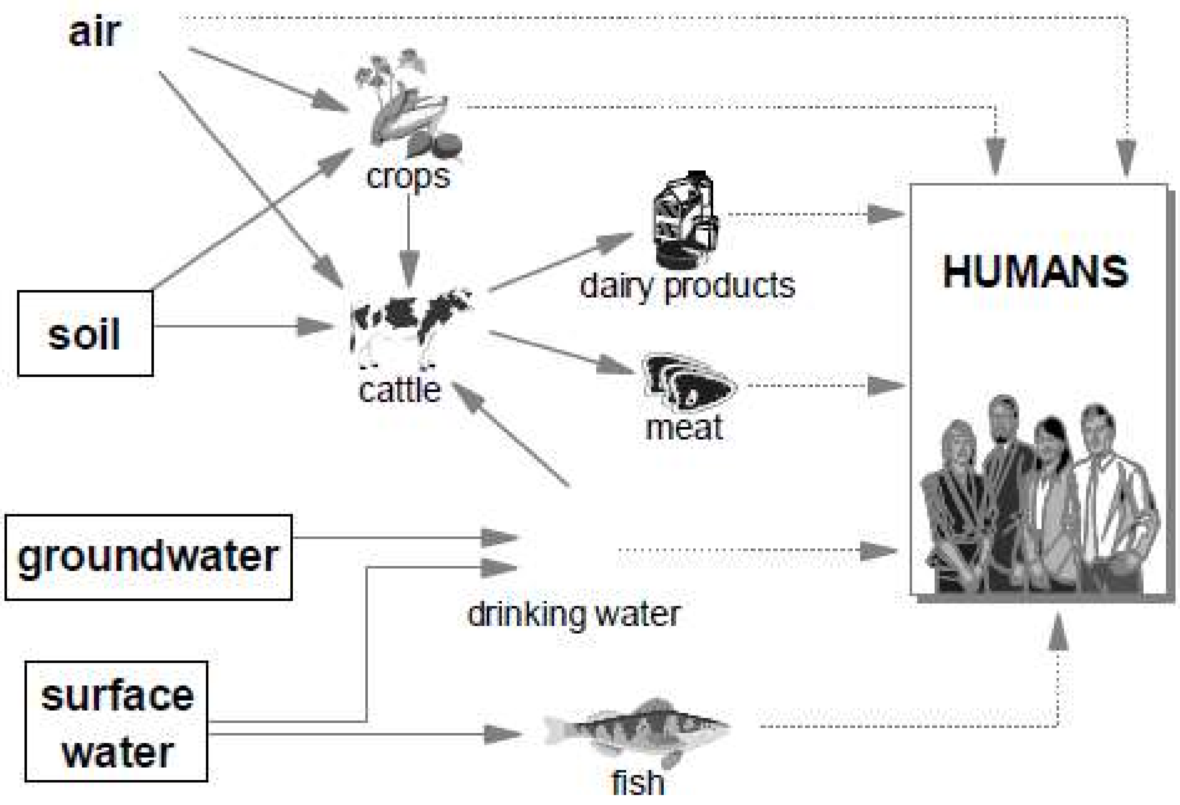




Stack height (m)	10
Stack diameter (m)	0.5
Gas exit velocity (m/s)	0.1
Gas exit temp. (C)	20

Stack height (m)	30
Stack diameter (m)	2
Gas exit velocity (m/s)	5
Gas exit temp. (C)	200

Man via the environment exposure Routes



Exposure man via the environment

- Both local and regional scale

- Concentration in intake media:
  - Food:
    - Crops (root and leaf)
    - Fish
    - Meat and dairy products (milk)
  - Air
  - Soil
  - Drinking water

- Review of exposure routes (food and drinking water) by Rikken (2004), RIVM Rapport 601900005

Air and soil

- Air
  - Modelled local and regional air concentrations are used
  - Continuous chronic exposure assumed
  - Model can be used for metals, assuming zero vapour pressure => 100% associate to aerosols

- Soil ingestion by humans not include in EUSES. For cattle soil ingestion is taken into account

Drinking water

- Highest concentration in either surface water or ground water is used as a source.

- Concentration ground water = Conc. pore water

- Only dissolved fraction is considered (complete removal of suspended particles assumed)

- Purification
  - It is assumed that the treatment processes for ground water have a negligible effect on the concentration
  - Estimation of purification factors for treatment of surface water not suitable for metals (based Kow, Henry's constant and Biodeg)

Food models

- Fish: $C_{fish} = BCF_{fish} \cdot C_{water}$
  - QSAR for BCF not suitable for metals, empirical values should be used

- Meat and milk: $C_{milk} = BAF_{milk} \cdot \sum C_i \cdot IC_i$ and $C_{meat} = BAF_{meat} \cdot \sum C_i \cdot IC_i$
  - Total intake via grass, soil, drinking water and air
  - BAF-QSARs are not suitable for metals
  - Instead empirical or modelled BAF-values should be used

Food models

- Plant uptake (root and leaf crops):
  - Model only valid for organic compounds
  - EUSES: same plant characteristics for grass and crops
  - Parameters represent a generic leafy crop and seem to characterise grasses
  - Empirical BCF values can be used to determine Croot and Cleaf outside EUSES
  - Alternatively empirical plant-water partition coefficients can be used as input to determine Croot (physical sorption)

  - Empirical BCF-values usually include local deposition, leave uptake etc.: Total uptake / Soil concentration

Food models

- The mechanisms of accumulation for metals in plant probably still not completely understood and difficult to model

- BCF depends on many factor such as soil characteristics and type of crop and is concentration dependent, =>large variation.

- Versluijs and Otte, 2001

$$\log[C_{v,dw}] = a_i + b_i \log[C_s] + c_i\, pH_{soil} + d_i \log[clay\%] + e_i \log[OC\%] + f_i[other\ factors]$$

  - Unfortunately, the statistical significance for the majority of the relationships was insufficient.

Food models, crops

- Approaches on which BCF/BTF to use
  - EUSES: one generic crop
  - BCF most critical crop
  - BCF consumption averaged

- Total exposure via food crops:

Uptake = Crop consumption x Conc in crop x Frac. Contaminated x Sorption

Conclusions

- EUSES for screening purposes
- Local air distribution does not represent sources with high stacks and heat content
- No site specific assessment
- Suitable for Neutral Organic Compounds
- For local and regional distribution of metals use vapour pressure zero and compartment specific partition coefficients (Kp)

Conclusions

- EUSES assessment of exposure [JB5] man via environment, following input is needed for metals:
  - Purification factors for removal of metals from surface water
  - Use metal specific BCFs for fish and
  - BAF/BTF-values for meat and milk for specific metals
  - Food crops: Cleaf and Croot should be calculated externally

Slide 37

JB5 Conclusie EUSES luchtverspreidingsmodel
Joost Bakker; 25/01/2017

2. Existing experience from modeling to monitoring based assessments Man via the Environment

REACH guidance on MvE in short and re-cap on metal existing AfA cases.

By Peter Simpson,
(ECHA)

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Indirect exposure of humans via the environment in REACH

Lessons learnt from the evaluation of applications for authorisation for inorganic substances

Peter Simpson, ECHA

Eurometaux scientific seminar on improving man via the environment scenario for inorganics with an emphasis on metals. 26th of January, 2017, Brussels

Overview

- Background
- REACH Guidance and links to EUSES/CHESAR tools
- Overview of previous applications for authorisation for inorganic substances
- Lessons learnt from evaluation by ECHA’s scientific committees
  - Refinements already widely practised
  - Further refinements
- Conclusions

Background

- Some authorisation applications for 'industrial uses' have reported significant associated health impacts in the general population from indirect exposure
  - Incidence of statistical cancer cases >>1 across EU (up to ~225)
  - Greatest impacts associated where uses are at many EEA sites
    - Linked to very large potentially exposed population
  - Underlying assessments sometimes, but not always, based on Tier I assumptions of exposure and exposed population size
  - Cause for concern?
    - Or consequence of the assumptions used to perform the risk assessment?
- RAC / SEAC have evaluated these impacts as uncertain
  - Refinements in assessment required in any review report
- Not a issue with every application!
  - Typically associated with non-threshold substances

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Impact in the general population

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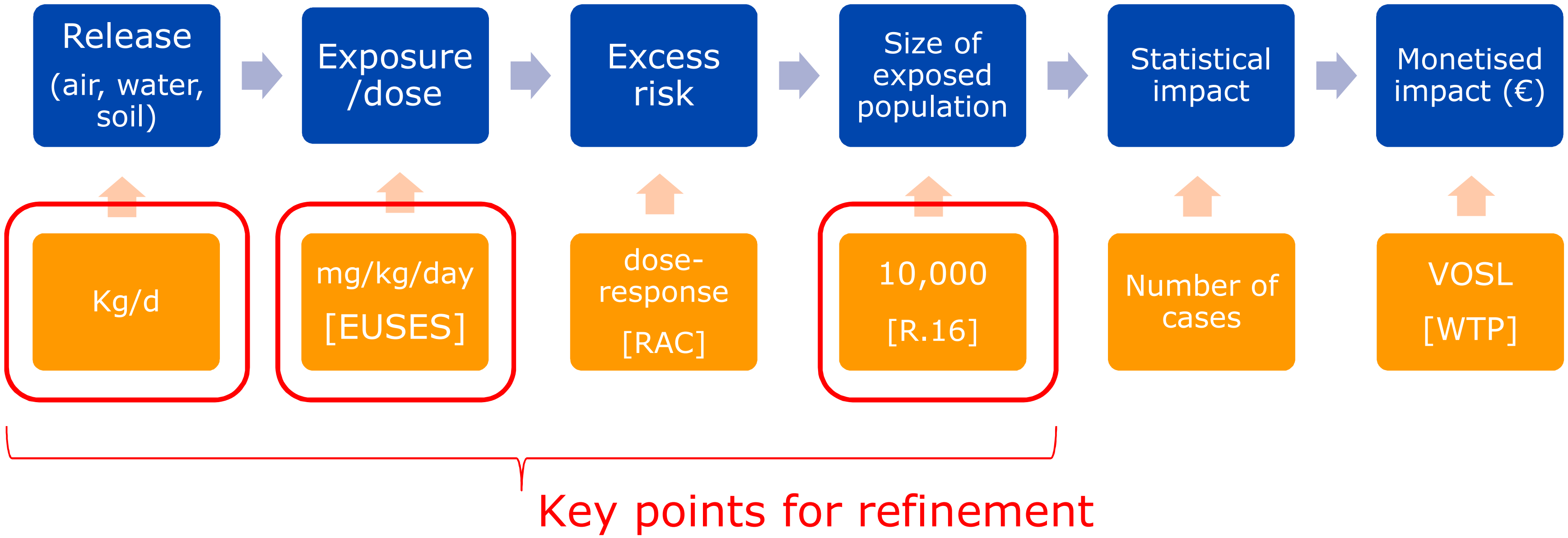

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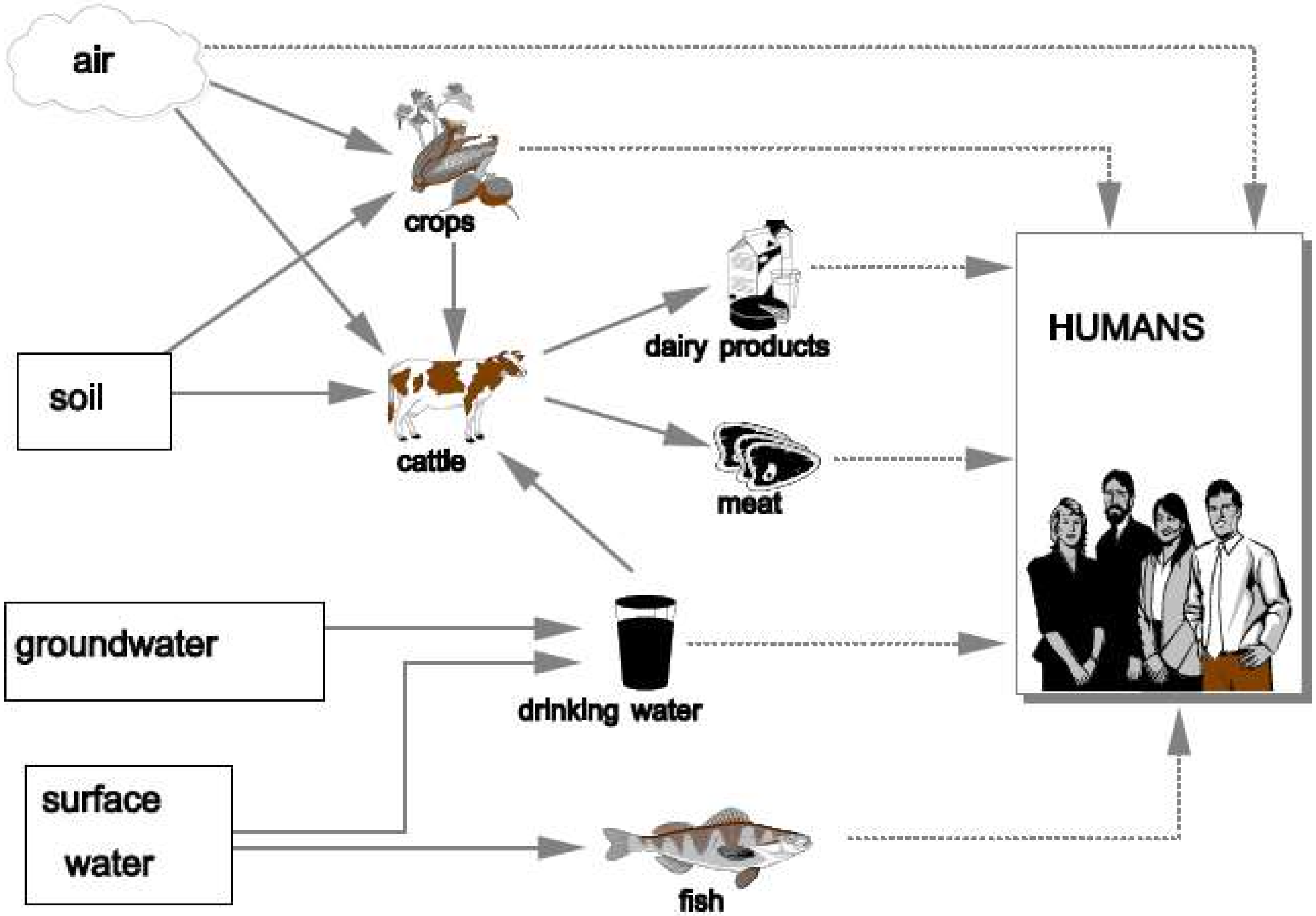
Section 6.2 (Risk characterisation)

Indirect assessment of humans via the environment



ECHA guidance for indirect assessment

- Default methodology in ECHA Guidance (R.16) is the EUSES model with default (Tier I) assumptions
- EUSES intended as a screening tool within a tiered risk assessment framework (RCR as trigger for refinement)
  - Estimated inhalation concentration (mg/m^3)
  - Estimated concentration in food products (mg/kg)
    - leaf crops (including cereals and fruit)
    - root crops
    - milk
    - meat
    - fish
    - drinking water
  - Estimated total human doses (mg/kg bw/day)
    - Standard inhalation rate and bodyweight assumptions
    - Standard food / water consumption rates

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EUSES/CHESAR – inputs

- Release rates – kg/day (air, water, soil)
- Substance properties for a **Tier I** (default) assessment

Parameter	Description	Source
MOLW	Molecular weight	Technical dossier – chapter 1.1
MP	Melting point of substance	Technical dossier– chapter 4
BP	Boiling point of substance	Technical dossier– chapter 4
VP	Vapour pressure of substance	Technical dossier– chapter 4[48]
SOL	Water solubility of substance	Technical dossier– chapter 4
K_{OW}	Octanol water partition coefficient of substance (not relevant for inorganics)	Technical dossier– chapter 4
Biode-gradability	Results of screening test on biodegradability. Not relevant for inorganic substances.	Technical dossier– chapter 5 See also Appendix A.16-3.2

- Other required data estimated with QSAR
  - Partition coefficients / degradation rates / bioaccumulation (BCF)
- **Tier I** modelling parameters reflect **typical** or **reasonable worst-case settings** – can be refined

EUSES/CHESAR – outputs

- Two "types" of PECs estimated
  - **PEC_{local}** – close to point source immediately after initial mixing
    - PEClocal,air – estimated 100m from point source (site boundary)
  - **$PEC_{regional}$** – steady-state concentration after distribution
- Very different temporal and spatial assumptions
- Both are "generic standard environments"
- Scales are intended to be interpreted together
  - Screening assessment for threshold substances
  - Is RCR <1 in both local and regional assessments?
  - Is RCR >1 in either or both of the assessments?
    - Refinement likely to be necessary!

Generic local assessment – common misinterpretations

"10 000 people are assumed to live within 100 metres of the site"

"The local scale is restricted to the population living within 100 metres of a site"

Assumption is:

- Site is associated with a standard town, where its releases result in exposure to the local population (10 000 people)
- All food / water is from affected area
- All population (and food) is exposed to the 'worst-case' concentration in air estimated to occur at the <u>site boundary</u>
- Crops, meat and milk are assumed to be from land subject to the mean deposition estimated within 1km radius of site

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R.16 - reality check!

It is clear that a generic indirect exposure estimation, as described by the calculations detailed in Appendix A.16-3.3.9, can only be used for screening purposes to indicate potential problems. The assessment should be seen as a helpful tool for decision making but not as a prediction of the human exposure actually occurring at some place or time.

ECHA R.16 guidance (version 3) – R.16.4.3.3 (p 65)

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Summary

1	Tier I assumptions in EUSES are intended for screening assessments
2	Local and regional Tier I assessments are "standard" environments that are intended to overestimate likely exposure; Tier I assumptions for local assessment are very conservative
3	Tier I local assessments will significantly overestimate exposure for the general population as most will not live 100 metres from a site, or consume all food from the local area
4	Tier I local assessments are particularly sensitive to release rates as only linear relationships are used to estimate exposure
5	Use of Tier I EUSES exposure estimates for impact assessment is likely, in many cases, to go beyond its intended use
6	Tier I assumptions will need refinement, in many cases, before EUSES estimates can be used in impact assessment

Inorganic substances on Annex XIV – adopted opinions (Jan '17)

Substance	Annex XIV entry number	Number of opinions agreed	Typical uses applied for
Diarsenic trioxide	8	5	• Zinc electrowinning • Ammonia manufacture • gold electroplating
Lead chromate pigments	11 & 12	12	• Non-consumer uses in paints for metal surfaces • Non-consumer uses in plastics
Lead chromate	10	1	• Decoy flares (military use)
Sodium chromate	22	1	• Inhibitor in ammonia adsorption cooling systems
Chromium trioxide	16	24	• Functional plating • Decorative plating • Production of coloured stainless steel • Conversion coating / passivation
Sodium dichromate	18	13	• Manufacture of sodium chlorate/chlorite • Inhibitor in ammonia adsorption cooling systems • Surface treatment • Metal refining
Potassium dichromate	19	7	• Optoelectronics • Conversion coating
dichromium tris(chromate)	28	3	• Surface treatment / conversion coating
strontium chromate	29	2	• Corrosion resistance in speciality paints / coatings
potassium hydroxyoctaoxodizincate dichromate	30	2	• Corrosion resistance in speciality paints / coatings
ammonium dichromate	20	2	• Photolithography
chromic acid	17	1	• Functional plating

Use of diarsenic trioxide in zinc electrowinning

- Two applicants:
  - Boliden Kokkola Oy; Nordenhamer Zinkhütte GmbH
  - Local population of 50 000 (3-4 km from site)
- Inhalation exposure from urban ambient monitoring
  - 0.007 µg/kg/day
- Oral exposure estimated using EUSES 2.1.2 and data on releases from site (local assessment assumptions)
  - Intake of 3.2 µg/kg/day
    - Leaf crops (68.9 %); Fish (28.9 %)
  - Refinement 1 - 1.3 µg/kg/day
    - Local data on leaf crop & fish consumption
    - Only 50% of leaf crops consumed were from local area
  - Refinement 2 - 10% of initial values)
    - Arsenic deposition in the nearest known agricultural area
    - Assumption that consumption rates for local leaf crops was insignificant
  - Final exposure estimate of 0.365 µg/kg/day
  - Excess risk of 6.1 x 10^{-4}; 25 statistical cancer cases over 70 yrs

Use of diarsenic trioxide in zinc electrowinning

- RAC noted in the opinion (adopted 06/09/2014) that:

'RAC considers that the exposure estimates derived by the applicant for the oral route (underpinned by modelling) are considerably more uncertain than the exposure estimates derived for the inhalation route (from monitoring).

RAC acknowledges that the use of EUSES is likely to overestimate the exposure via the oral route in this application … and that further refinement of model parameters or the use of alternative models or techniques may allow a more definitive description of the exposure to man via the environment…

…However, despite these limitations, RAC considers that the combined exposure estimate …… is suitable for the use as a worst-case in impact assessment by SEAC.'

Use of diarsenic trioxide in zinc electrowinning

- Conditions in decision:

‘When submitting the review report referred to in Article 61(1) of Regulation (EC) No 1907/2006 the holder of the authorisation shall provide a more refined and thereby improved exposure assessment for both workers and man via the environment.’

Inorganic substances on Annex XIV – adopted opinions (Jan ’17)

Substance	Annex XIV entry number	Number of opinions agreed	Typical uses applied for
Diarsenic trioxide	8	5	• Zinc electrowinning • Ammonia manufacture • gold electroplating
Lead chromate pigments	11 & 12	12	• Non-consumer uses in paints for metal surfaces • Non-consumer uses in plastics
Lead chromate	10	1	• Decoy flares (military use)
Sodium chromate	22	1	• Inhibitor in ammonia adsorption cooling systems
Chromium trioxide	16	24	• Functional plating • Decorative plating • Production of coloured stainless steel • Conversion coating / passivation
Sodium dichromate	18	13	• Manufacture of sodium chlorate/chlorite • Inhibitor in ammonia adsorption cooling systems • Surface treatment • Metal refining
Potassium dichromate	19	7	• Optoelectronics • Conversion coating
dichromium tris(chromate)	28	3	• Surface treatment / conversion coating
strontium chromate	29	2	• Corrosion resistance in speciality paints / coatings
potassium hydroxyoctaoxodizincate dichromate	30	2	• Corrosion resistance in speciality paints / coatings
ammonium dichromate	20	2	• Photolithography
chromic acid	17	1	• Functional plating

Use of chromium trioxide for functional chrome plating

- Seven joint applicants – for uses further down the supply chain – application by an upstream actor
  - Use estimated to take place at 1,590 sites
  - Locally exposed population across EU of 15 900 000
- Only inhalation route considered in application
  - 90^{th} percentile of available release data used (17 sites – 1%)
  - EUSES used to estimate PEClocal,air (@100 metres)
  - 2.85×10^{-3} µg/m^3 – equivalent to excess risk of 8.3×10^{-5}
- Applicant considered the release to wastewater were negligible – oral exposure/impact not estimated
- Impact on humans exposed by the environment
  - local population of 10,000 people at each site
  - 225 statistical cancer cases in EU over 12 years

Use of chromium trioxide for functional chrome plating

- RAC noted in its opinion (adopted 16/09/2016):

'RAC acknowledges that Cr(VI) will transform rapidly in the environment to Cr(III) under most environmental conditions. This [was discussed] in the EU RAR for chromate substances (EU RAR 2005), and will reduce the potential for indirect exposure via the environment, particularly via the oral route.

'RAC notes that the applicant's use of a 90^{th} percentile value for estimating releases to atmosphere is likely to overestimate the $PEC_{local,air}$ at many of the sites undertaking this use.'

'RAC notes that the default assumptions in EUSES for local assessment estimate [exposure based on] a PEC [estimated] 100m from a point source. This, in general, is likely to overestimate exposure for the majority of the people living in the vicinity of a site.'

Use of chromium trioxide for functional chrome plating

- SEAC noted in its opinion (adopted 16/09/2016):

'As the methodologies used by the applicant (particularly the generic exposure assessment for the general population using the EUSES model) focus on individuals or locations with a high potential for exposure, the overall number of cases is likely to have been significantly overestimated.

In the absence of more refined estimates, RAC and SEAC have based their opinion on the assessment presented by the applicant. However, the health impacts should not be seen as equivalent to the human health impact that will occur if an authorisation for this use is granted.

Use of chromium trioxide for functional chrome plating

- Proposed conditions and monitoring arrangements in opinion:

‘The assessment of indirect exposure and risk to humans via the environment should be refined beyond the default assumptions outlined in ECHA guidance and the EUSES model with specific data appropriate to a more refined analysis.

ECHA
EUROPEAN CHEMICALS AGENCY

Refined approaches already practiced

- R.16 guidance is **already clear** that refinement to default Tier 1 approaches might be required.

… if either local or regional-scale assessments indicate a risk, there is usually a need for refinement

*When refinement is necessary, it should initially be considered if the **release estimates are realistic**. Subsequent refinements, if needed, should focus on the **concentrations in relevant environmental compartments***

Refined modelling of inhalation exposure

- Used in many applications
- Plume modelling
  - Vlisco (TCE)
  - Inhalation exposure
  - Could be extended to deposition rates
- Defining the extent of 'impact zone' important

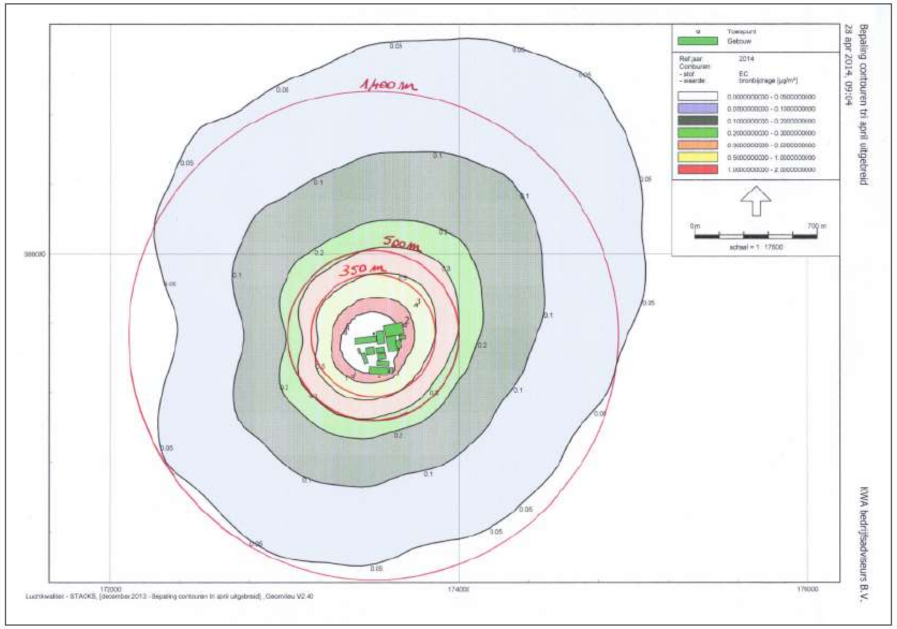


Figure 10: TCE concentrations in the area surrounding the Vlisco site

Table 31. Calculation of exposure of man via the environment using an alternative exposure model

Distance from Vlisco (circles)	Man via environment – inhalation (Geomilieu)	Man via environment – oral (EUSES)	# people[21]
Vlisco to ≤ 350m	0.002 to 0.0005 mg/m^3	7.297E-4 mg/kg bw/day	3,676
> 350 to ≤ 500m	0.0005 to 0.0003 mg/m^3	7.297E-4 mg/kg bw/day	8,521 – 3,676 = 4,845
> 500 to ≤1400m	0.0003 to 0.00005 mg/m^3	7.297E-4 mg/kg bw/day	51,908 – 8,521 = 43,387
> 1400m	< 10% of lowest background conc. in the Netherlands (0.0008 mg/m^3)[22] ➔ not taken into account any more		

‘central tendency’ versus ‘worst case’

- Tendency when undertaking risk assessment is to use (reasonable) worst case assumptions – 90th percentile
  - Frequency, duration, exposure, intake rates
  - Exposed population
- Impact assessment tends to need ‘bigger picture’
- Impact assessment based on worst case assumptions will overestimate the impacts from a use
  - Exposures lower for the majority of workers
  - Not all locally exposed general population will be 100 m from a site
  - Releases from different sites (and population exposed) will not all be the same

ECHA SEA guidance

In order to be able to quantify the impacts upon human health, a number of types of data are likely to be needed:

- Quantitative estimates of the relationship between individual exposure and incidence of a health effect (dose-response)
- Assessment of exposure, including duration and frequency
- A measure of the health impact (e.g. lost life years)
- An estimate of the total population exposed (and if possible the **distribution of exposures** within that population).

3.4.4.4 Quantitative assessment of impacts

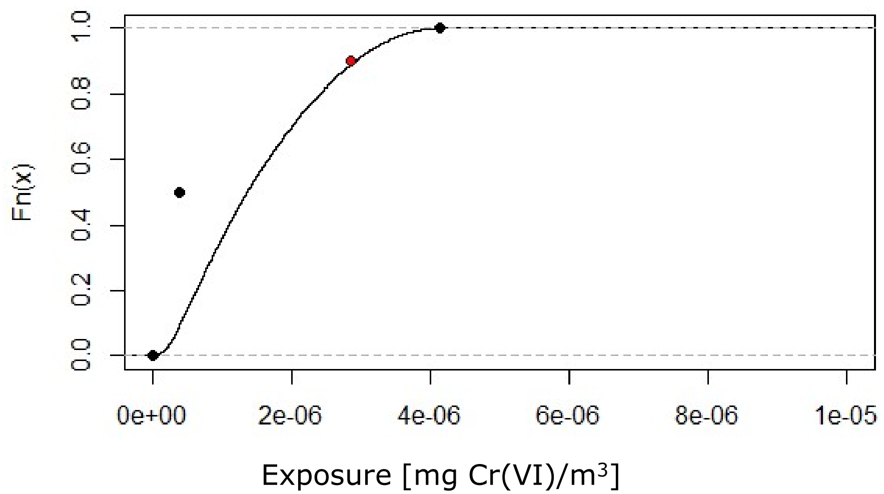
‘central tendency’ versus ‘worst case’

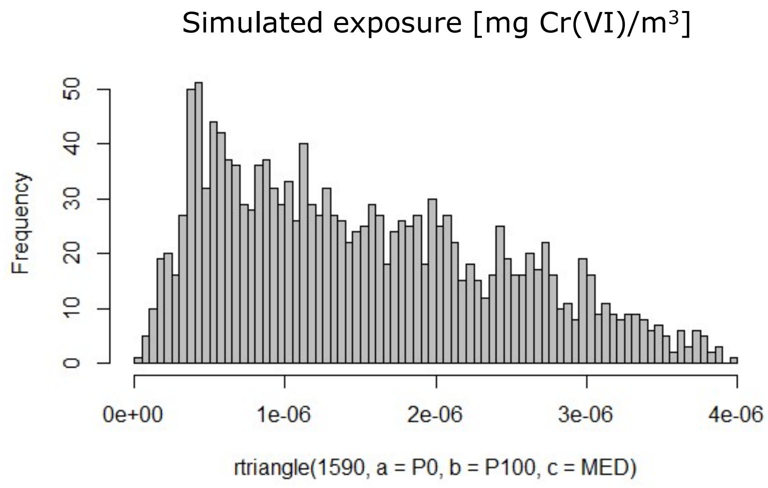
- Consider an assessment of multiple sites across the EU
  - Potentially 1 000s of sites
  - Site-specific variability in terms of release, exposure and population
  - Generic assessment based on worst case will result in significant impacts
  - What kind of refinements could be explored?
  - Are probabilistic approaches a useful tool?

No of Sites	Reporting Year	Range $Clocal_{air,ann}$ [mg Cr(VI)/m^3]	Arithmetic Mean [mg Cr(VI)/m^3]	Geometric Mean [mg Cr(VI)/m^3]	90th Percentile [mg Cr(VI)/m^3]
17	2010-2013	4.14E-06 – 2.69E-09	9.58E-07	3.83E-07	2.85E-06

Incorporate the variability in releases

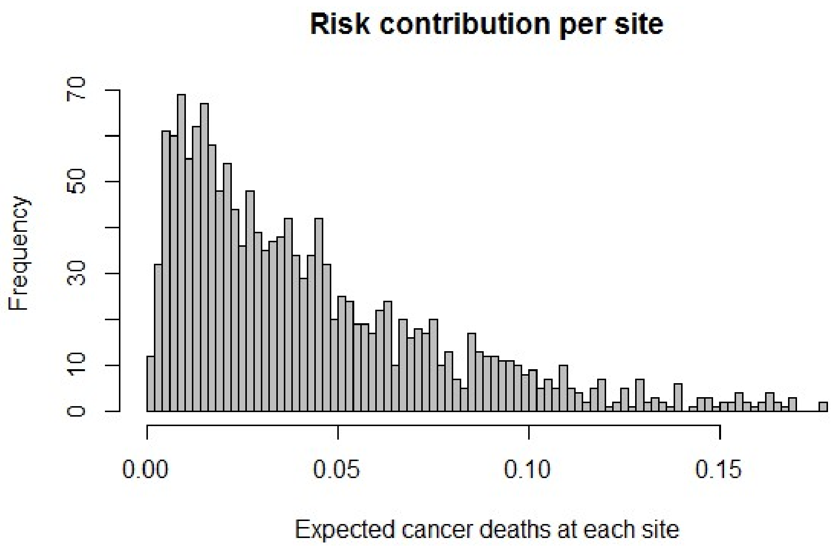
- A distribution can be fitted to simulate the exposure 100 metres from point source across the 1,590 sites
- Assumes that the data provided are representative
- Exposure is lower at 90% of sites!





What about number of people exposed?

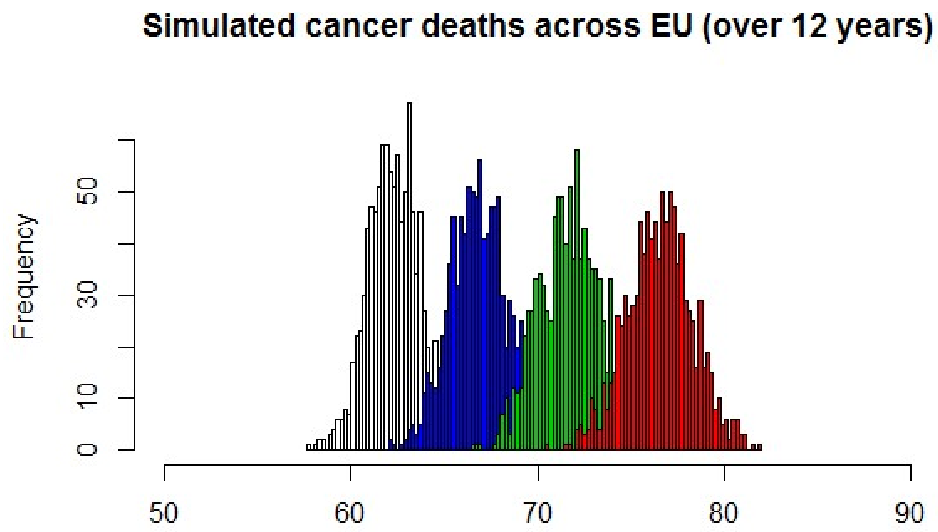
- Applicant used a default value of 10,000 people exposed per site (to the concentration estimated 100 metres from point source)
- Combined with the 90th percentile exposure value this leads to ~225 additional cancer deaths over a 12-year period
- Default is not likely to be appropriate at all sites. What if the population at risk was any number between 1,000 and 10,000?



- Re-run many times to build "virtual worlds" (10,000)
- Sum across one world yields expected cases
- Distribution over worlds gives an idea about the variability in expected cases

Refined estimate of impact

- These simple refinements result in 60 to 80 cancer cases
- ~25% of the impact estimated in the application



Still uncertain and precautionary

- Minimum local population of 1,000 likely a significant overestimate for some sites
- Factor of 0.5 used to estimate Cr(VI) from Cr_{total} – could be >0.95
- Exposure assessment assumes that all particles are respirable
- Conversion of Cr(VI) to Cr(III) in the atmosphere after release not addressed

Conclusions

- Indirect exposure assessment is a key element of the impact assessment for many for non-threshold AfA
  - Do the benefits of use outweigh the risks?
- Limitations of default methodologies, in certain circumstances, are already clearly acknowledged in Guidance
  - Issues observed are associated with the application of screening tools beyond their intended scope
- Significant potential to refine the Tier I assessment undertaken by EUSES, where this is necessary, using existing tools
- Refined assessments should initially focus on improving estimates of releases to the environment

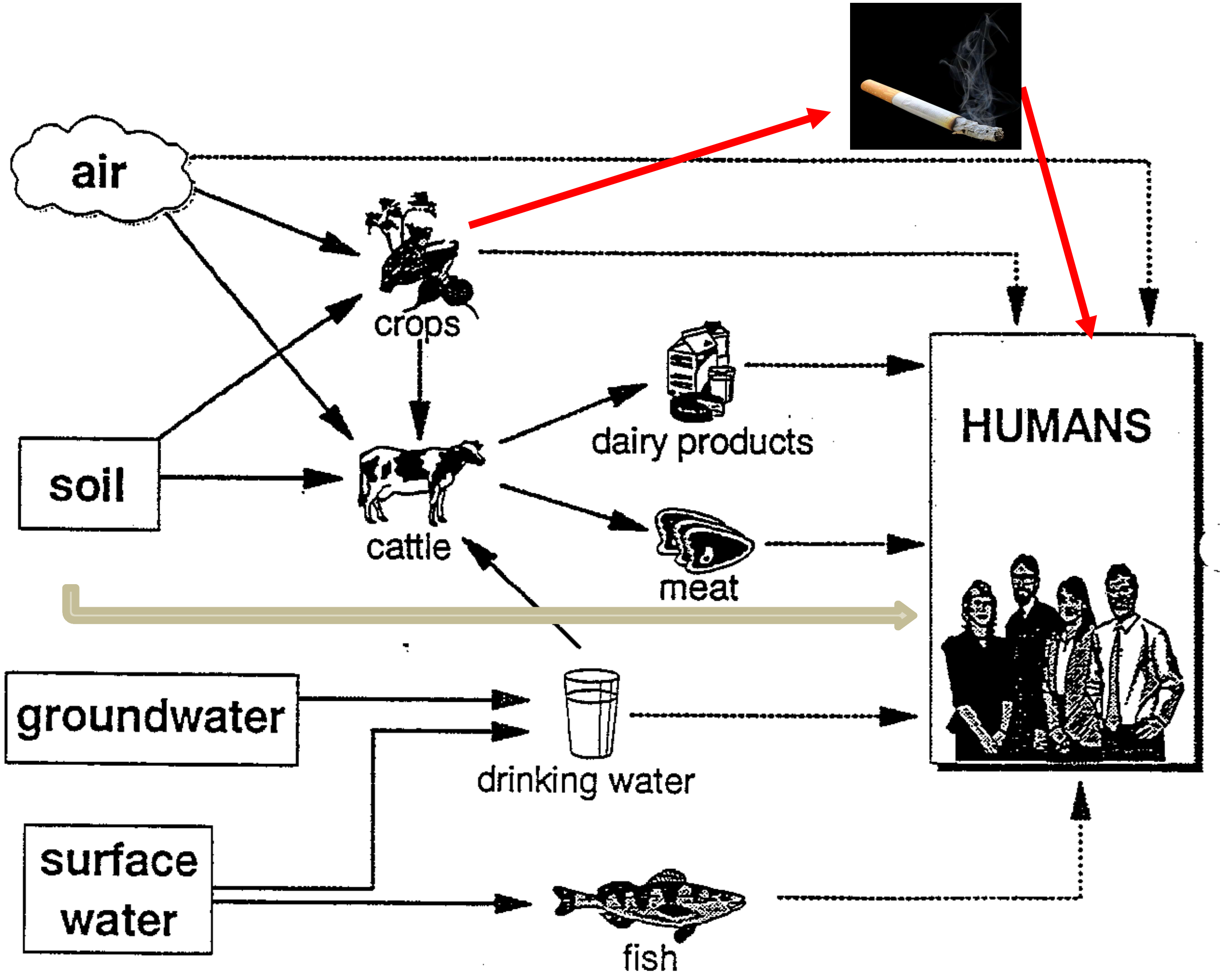
international zinc association

2. Existing experience from modeling to monitoring based assessments Man via the Environment

MvE scenarios in REACH registration files for metals, the Cd case

By Frank Van Assche,
(IZA)

Exposure of man via the environment



Issues with modelling : dietary

- Dietary habits
  - Bio-availability of metal in different food sources
- Soil - plant transfer
  - Local or generic produce?
  - BCF's? Species?
- Fish – meat?
- Drinking water conditions, local?

↓

- Monitoring of dietary intake: more realistic dietary sources
  - Absorption factors?

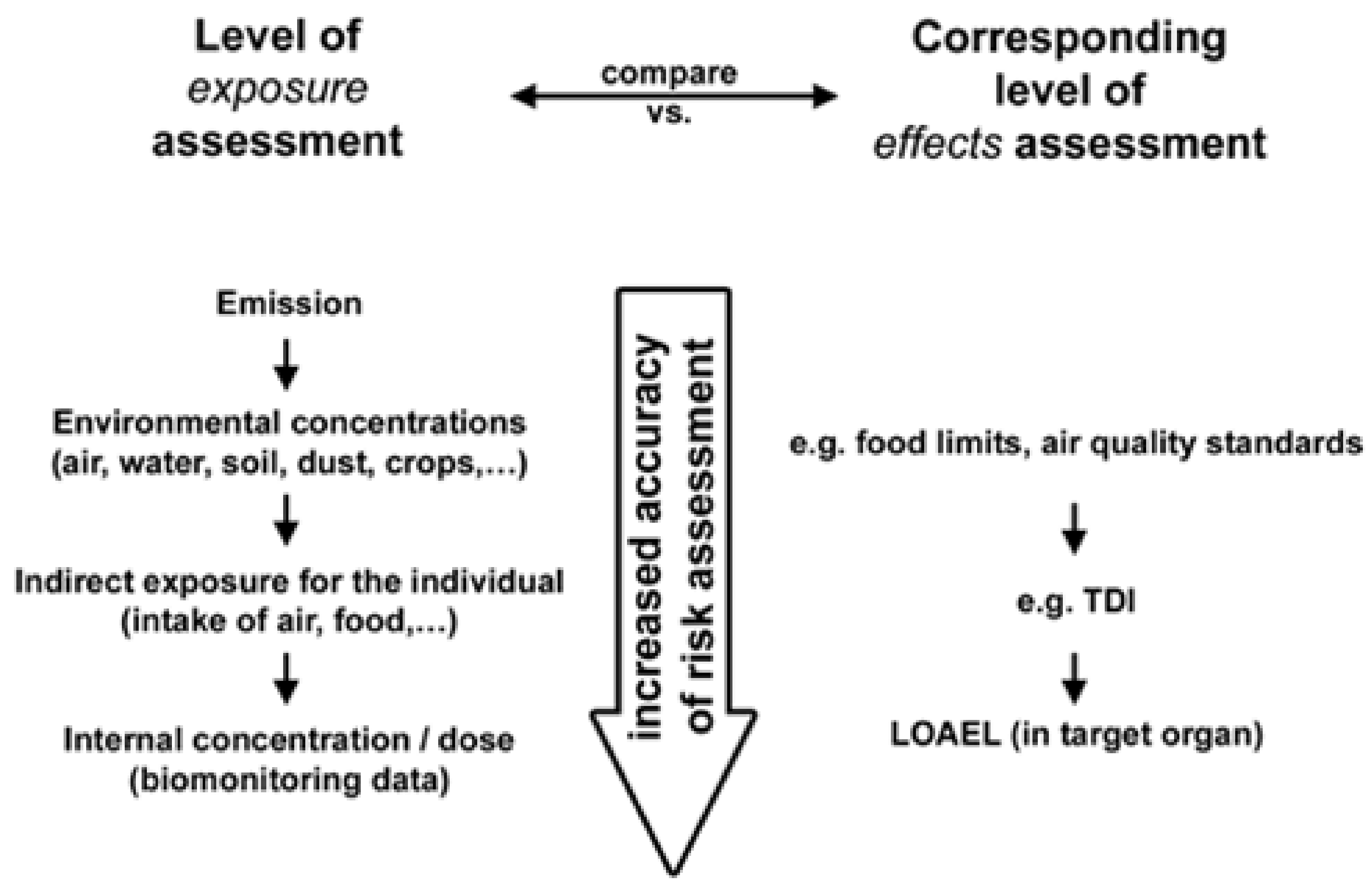
↓

- Bio-monitoring of internal exposure (all routes)

Issues with modelling : inhalation

- Modelling emissions
  - Distance and position to source
  - Fugitive emissions?
  - Environmental conditions?
  - Particle sizes?
- Monitoring of ambient air levels: integration of all sources
  - Point and diffuse sources
  - Real conditions at place of exposure
- Bio-monitoring of internal exposure (all routes)

Refinement of the assessment



Source: HERAG fact sheet indirect exposure / consumer exposure

MvE exposure to metals: main sources

metal	main exposure	comments
Cd	Dietary	plant uptake from soil dominates; smoking may be significant source
Cu	Dietary, drinking water	Deposition on crops may be important ; Drinking water depends on corrosivity
Pb	Dietary, drinking water	Possible influence by historical uses e.g. fuel, soldered cans, water pipes,.. Smoking may be significant source
Zn	Dietary	Intake is at recommended daily values

MvE exposure to metals: general and specific

- General:
  - dietary, (drinking water)
  - smoking
- Specific (local):
  - Inhalation (if significant emission to air)
  - If local produce consumption
    - Vegetables (fruits)
  - Soil/dust ingestion (when historical contamination)
    - outdoor soil versus indoor dust levels

Environmental exposure to Cd

- Well documented case (ESR-RA, 2008, ⇨…)
  - Exposures based on measured levels
  - Toxicokinetics well-known
  - Biomonitoring parameters well established
- Sources
  - Dietary
  - Smoking
  - Inhalation?
  - Soil/dust ingestion?

Monitored data: general population

- Dietary intake studies EU – countries
  - Adults:
    - 14 µg Cd/d (50P)–28.7 µg Cd/d (95P); Gastro-intestinal absorption: 3%
  - Children:
    - 8 µg Cd/d; G-I absorption: 5%
- Drinking water:
    - <1µg Cd/l ; 2 l/d consumption
- Inhalation: ambient air
  - Rural-urban (max): 1-5 ng Cd/m^3
    - Daily inhalation 20m^3 (adults), 10m^3 (children); absorption rate: 25%
- Soil/dust exposure (children)
    - Cd content dust 7mg/kg; 100mg/d intake; absorption rate 5%

Calculations: general population

source	calculations	Cd uptake (µg Cd/d)
Dietary	8 µg/d * 0.05 (children) 14 µg Cd/d * 0.03 * (adults) (27.8 µg Cd/d * 0.03)	0.40 0.42 (0.83)
Air	0.005 µg/m3 * 10 m3 * 0.25 (children) 0.005 µg/m3 * 20 m3 * 0.25 (adults)	0.013 0.025
Drinking water	<1 µg/l * 1 l/d * 0.05 <1 µg/l * 2 l/d * 0.03	< 0.05 < 0.06
Soil and dust	7mg Cd/kg * 0.1 kg/d * 0.05 (children)	0.035
TOTAL		**< 0.50 (children)** **< 0.51 (adults)**

Specific scenarios

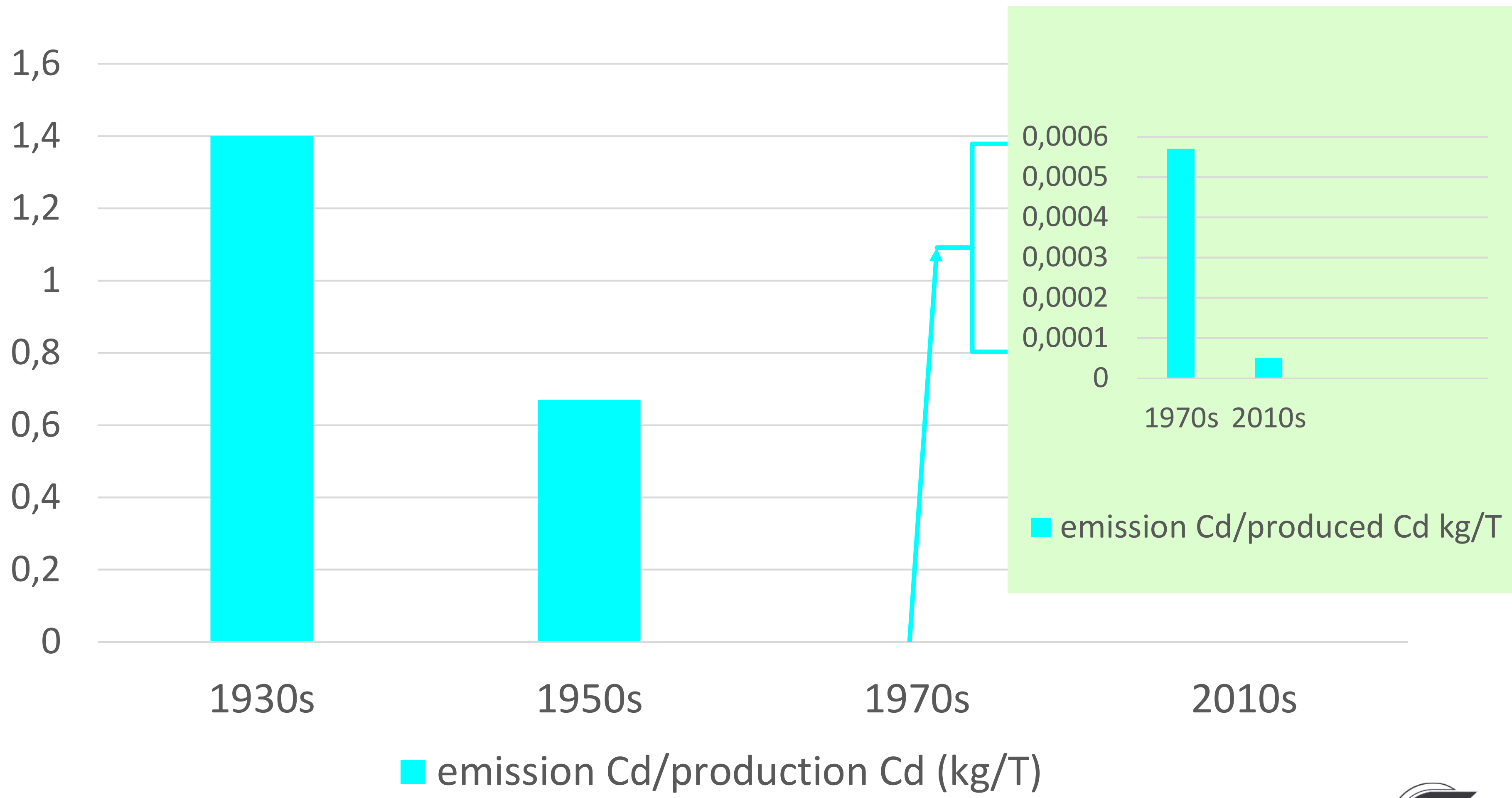
- Adults with depleted Fe- (Ca-, Zn-) stores:
  - Absorption rate: 6%
- Near point sources/historical contaminated area
  - Ambient air: 10 ng Cd/m3
  - Use 95P dietary intake
  - Soil/dust content: 15mg Cd/kg
- Smoking
  - 20 cigarettes @1-2 µg Cd/cig; inhaled fraction 10%; absorption rate 25-50%

Calculations: general population, Fe-depleted stores*

source	calculations	Cd uptake (µg Cd/d)
Dietary	14 µg Cd/d * 0.06 * (adults) (27.8 µg Cd/d * 0.06)	0.84 (1.66)
Air	0.005 µg/m3 * 20 m3 * 0.25 (adults)	0.025
Drinking water	<1 µg/l * 2 l/d * 0.06	< 0.06
TOTAL		**< 0.93 (adults)**

* Fe-depletion is not to be considered a continuous state

exposure near point sources: progressive emission control



Cd emissions to air (T/a) in the EU, 1990s ⇨ 2007 ⇨ 2010

Source/YEAR	Early 1990s* (EU 12)	2007 (EU 27)**	2010 (EU 27)**
Fossil fuel combustion	49.4	7.4	2.2
Iron & steel production	24.2	3.7	4.3
Non ferrous metals production	13.6	3.2	2.1
Cadmium production	1-3.9	0.44	/
Cement production	7.0	0.62	0.22
Other sources		4.3	4.2
TOTAL	**98**	**20**	**13**
*Natural emissions**	*~=15*	*~=15*	*~=15*

*ERL 1993; **e-PRTR

Population near point source

source	calculations	Cd uptake (µg Cd/d)
Dietary	(14 µg Cd/d * 0.03) (adults) 27.8 µg Cd/d * 0.03	(0.42) 0.83
Air	0.01 µg/m3 * 10 m3 * 0.25 (children) 0.01 µg/m3 * 20 m3 * 0.25 (adults)	0.025 0.050
Drinking water	<1 µg/l * 1 l/d * 0.05 <1 µg/l * 2 l/d * 0.03	< 0.05 < 0.06
Soil and dust	15 mg Cd/kg * 0.1 kg/d * 0.05 (children)	0.075
TOTAL		**< 0.98 (children)** **< 0.94 (adults)**

Calculations: smokers

source	calculations	Cd uptake (µg Cd/d)
Dietary	14 µg Cd/d * 0.03 (27.8 µg Cd/d * 0.03)	0.42 (0.83)
Air	0.005 µg/m3 * 20 m3 * 0.25	0.025
Drinking water	<1 µg/l * 2 l/d * 0.03	< 0.06
Smoking	20 cigarettes/day * 1-2µg Cd/c * 10% inhaled * 0.25-0.5	0.5-2.0
TOTAL		**< 1.0 - 2.5 (adults)**

Conversion of Cd intake to internal Cd exposure

- Cd-U is measure of internal systemic exposure
- Nordberg-Kjellström model:
  - Continuous uptake of 1µg Cd/d ~= Cd-U of 0.5µg Cd/d at age of 50

scenario	µg Cd/d intake	Cd-U (µg/d) calculated	Cd-U measured (µg/d or µg/gC) - 50P	Cd-U measured (µg/d or µg/gC) – 90 or 95P
General population; children	0.50	0.25	0.08 (DE; 2003-2006)* 0.07 (EU-17; 2014)**	0.22 (DE; 2003-2006) 0.22 (E-17; 2014)
General population; adult non smokers	0.51	0.25	0.21 (DE; 1998)*	0.77 (DE; 1998)
General population; smokers	1.0 – 2.5	0.5 - 1.25	0.33 (DE; 1998)*	1.3 (DE; 1998)*
General population, smok/non-smok			0.22 (EU-17; 2014)**	0.62 (EU-17; 2014)**

**Schulz et al 2007; ** Democophes 2014*

Summary and conclusions

- For MvE scenarios monitored data will provide more realistic assessments
- If available, bio-monitoring of exposure is best
- Specific sub-populations may be considered
- Most recent monitored data should be used to assess the current situation
- In general, the dietary route is most relevant for metals
- Part of exposure is related to natural metal background
- Historical contamination may be part of the exposure at older industrial sites

2. Existing experience from modeling to monitoring based assessments Man via the Environment

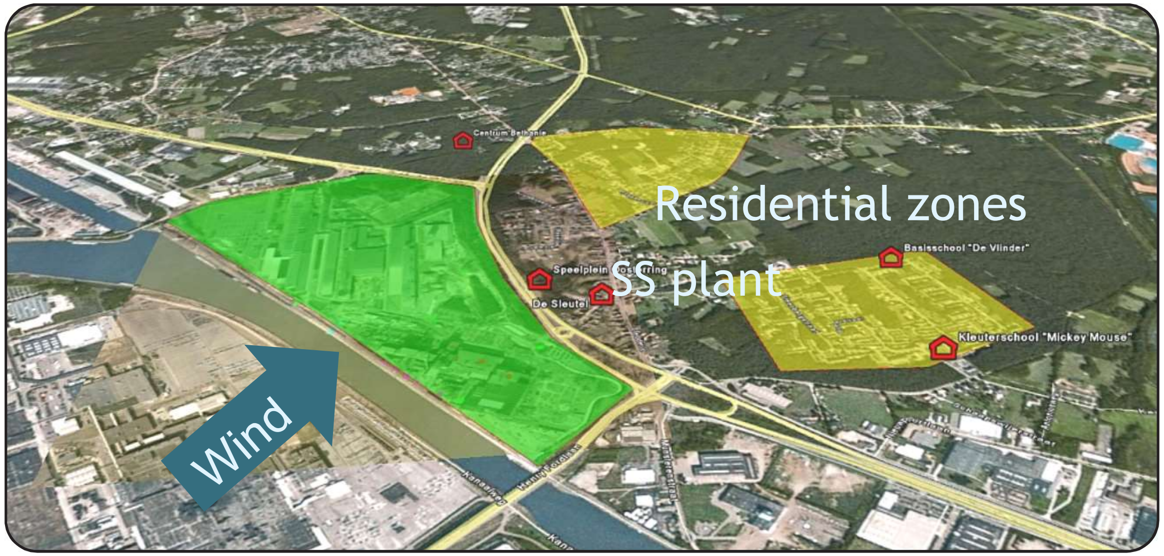
A site specific Risk Assessment on the Impact of Ni on the population surrounding a stainless steel production site

By Katleen De Brouwere,

(VITO)

CONTEXT

Health impact on people living in the close neighboorhood of the SS plant in Genk (B) ?



1. How is MvE exposure for this site addresses under REACH CSR (Ni dossier) ?
2. Site specific Risk assessment : forward modelling environment → health
3. Biomonitoring study in residential area

vito

1. ASSESSMENT UNDER REACH FOR THIS STAINLESS STEEL PLANT

Source : Ni CSR dossier (update 2015)

- Inhalation exposure : based on monitoring data
    - 17 ng Ni /m^3 (year average of one monitoring station, at time of data collection in 2012)
    - $RCR = {}^{exposure}/_{DNEL}$
    - DNEL/DMEL for Ni (Ni REACH dossier): 20 ng/m^3
    - → RCR for this site = 0,85 < 1
- Oral exposure (food and dust ingestion)
    - Generic approach, based on Tier 1 modelling and EUSES defaults
    - not elaborated in detail, since the condition of the generic exposure scenario for inhalation is reported to sufficiently protective also for the oral route (RCR << 1)

2. SITE SPECIFIC RISK ASSESSMENT

Context of this study

» outside REACH

» in framework of local public concern around the site (authorities and local communities in Genk)

» Study performed in 2008-2009

Which site specific aspects considered?

1. Speciation of Nickel in ambient dust around the SS plant
2. Spatial differentiation in function of wind direction, distance and population density
3. Site specific monitoring data in environmental media

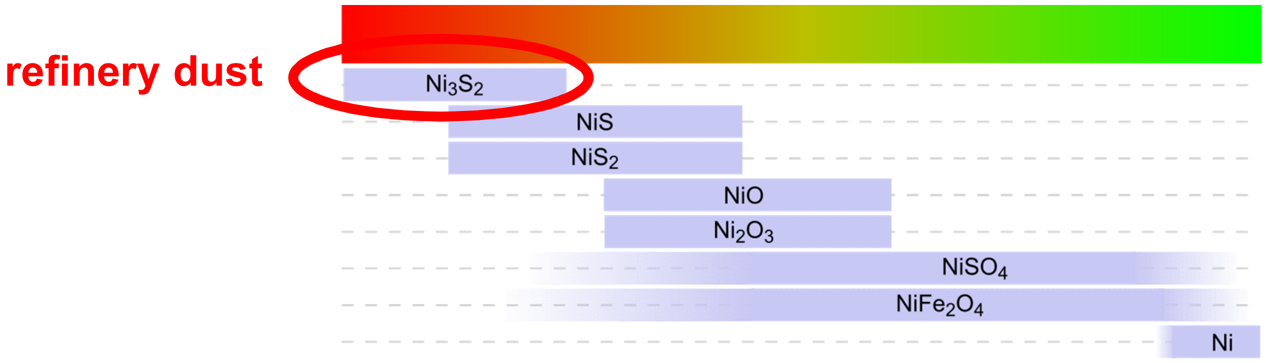
vito

2. SITE SPECIFIC RISK ASSESSMENT: APPROACH

1. Speciation of nickel in suspended dust around SS plant

» Ni dust consists of a wide range of Ni compounds:
metallic form, sulfides, oxides, soluble compounds, ...

» Some of these are more toxic/carcinogenic than others



» Composition of Ni dust strongly depends on the source / production process

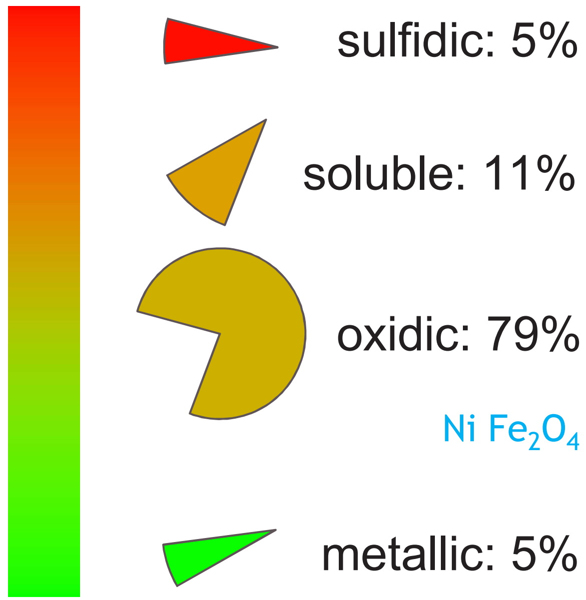
» most risk values for carcinogenic effects of Ni are based on occupational studies from Ni refineries

≠ stainless steel production

1. Speciation of nickel in suspended dust around SS plant

- Techniques for speciation of Ni compounds:
  - Chemical techniques
    - Zatka procedure
    - discerns 4 groups of Ni compounds:
      metallic – sulfidic – oxidic – soluble
  - Physical techniques
    - “XANES”, “XRD”, “EDX” procedures
    - can discern individual Ni compounds
    - only give a partial or qualitative image of the dust composition
    - need large quantities of Ni dust for accurate analysis

Ni speciation in ambient air PM in residential area around SS plant

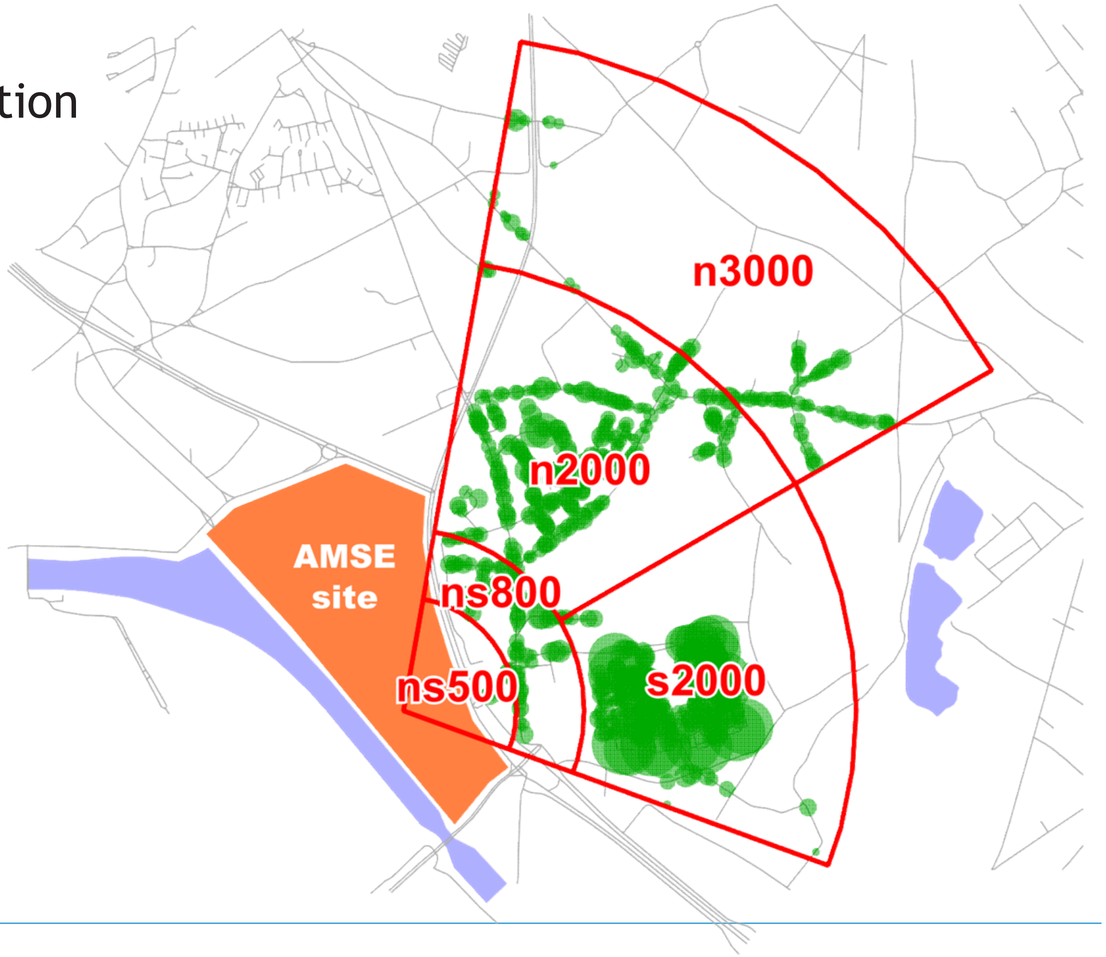


Tirez et al. 2011; Speciation and fractionation of nickel in airborne particulate matter: comparison between selective leaching and XAS spectroscopy. Journal of Analytical Atomic Spectrometry; Vol 26: 3; 517-527

2. Spatial differentiation

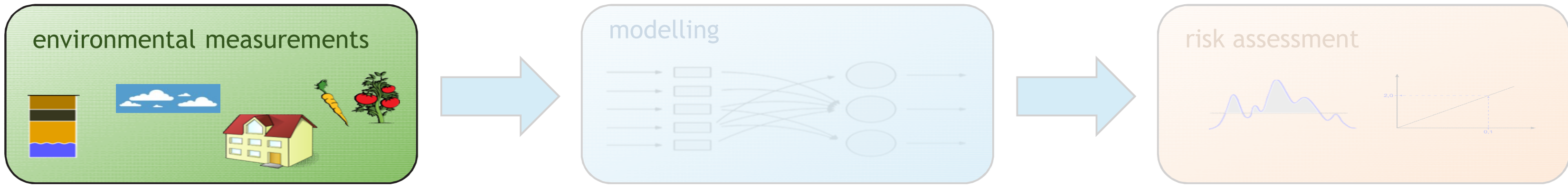
Spatial differentiation in exposure (oral, inhalation route) based on

- » distance
- » wind direction
- » population density



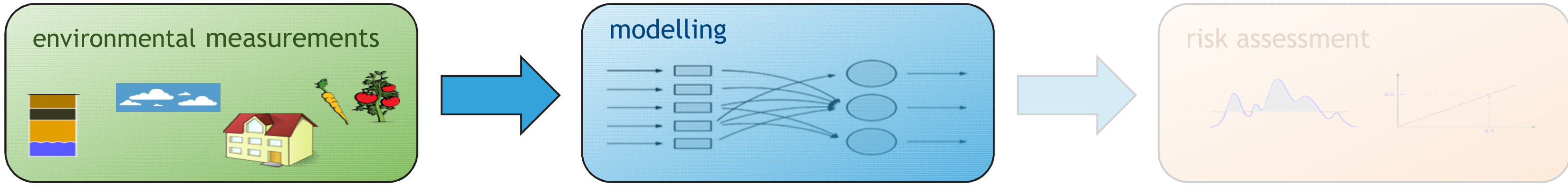
2. SITE SPECIFIC RISK ASSESSMENT: APPROACH

3. Monitoring data around the site



- Environmental measurement campaign in autumn 2008
  - suspended particulate matter in outdoor & indoor air
  - indoor deposited dust: wipe tissues & vacuum cleaner bag
  - soil near the residences
  - street dust in often frequented places
  - limited measurements on vegetables & fruits
- Air quality Measurements available from VMM (Flemish Environment Agency)
  - 4 measuring stations in the neighbourhood
  - past measurement record allow to determine time trends

2. SITE SPECIFIC RISK ASSESSMENT: APPROACH

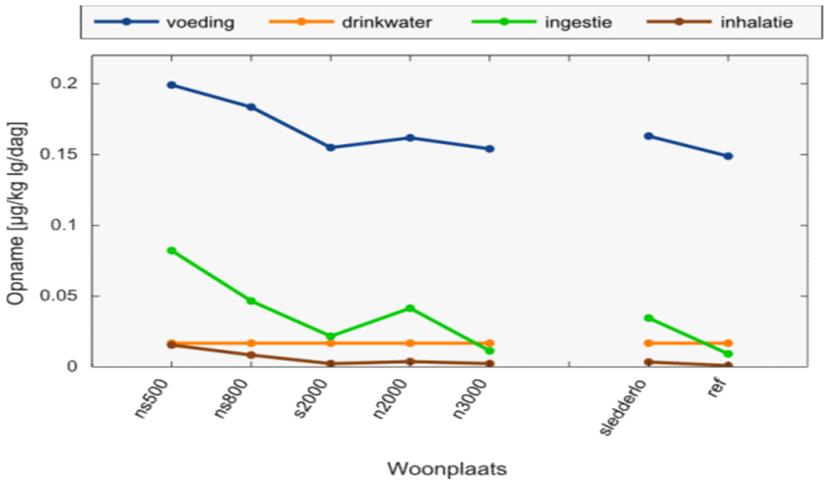


- Exposure model: Calculate human intake & health risk from environmental concentrations:
  - systemic exposure
    = sum of food & drinking water consumption, soil & dust particle ingestion
    - Intake from food:
      - local and non-local component
      - Belgian food basket (data WIV, 2004) applied
  - Inhalatory exposure
  - Predictions for oral and inhalation exposure for different population groups (age classes and time-activity patterns) and zones in relation to distance/wind direction of plan; attribution of monitoring data to appropriate zones (spatial)

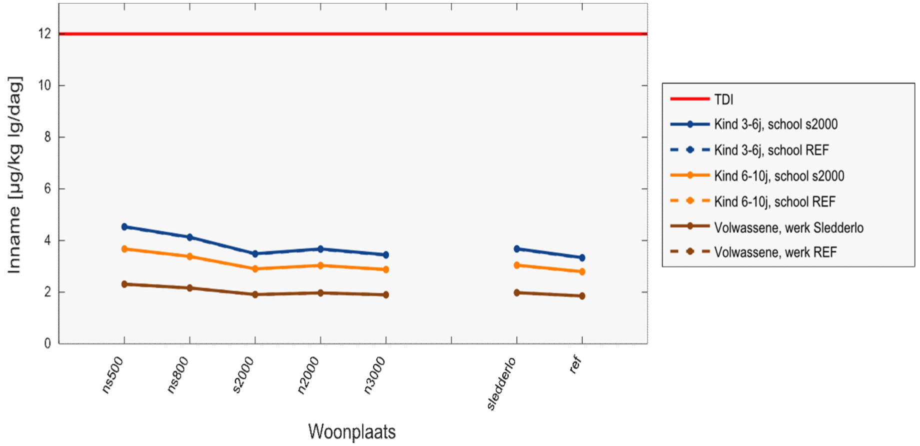
2. SITE SPECIFIC RISK ASSESSMENT: RESULTS

Systemic exposure (= oral + inhalation)

Ni intake child (3-6 years)



systemic: TDI Ni $_{sulfate}$: 12 µg/kg bw (WHO, 2006)



2. SITE SPECIFIC RISK ASSESSMENT: RESULTS

inhalation exposure - carcinogenic effects

» Carcinogenic effects = the additional risk of developing cancer over the whole lifespan, expressed per µg/m³ Ni

mathematical

air concentration

×

unit risk

=

additional risk caused by Ni

example

20 ng/m³

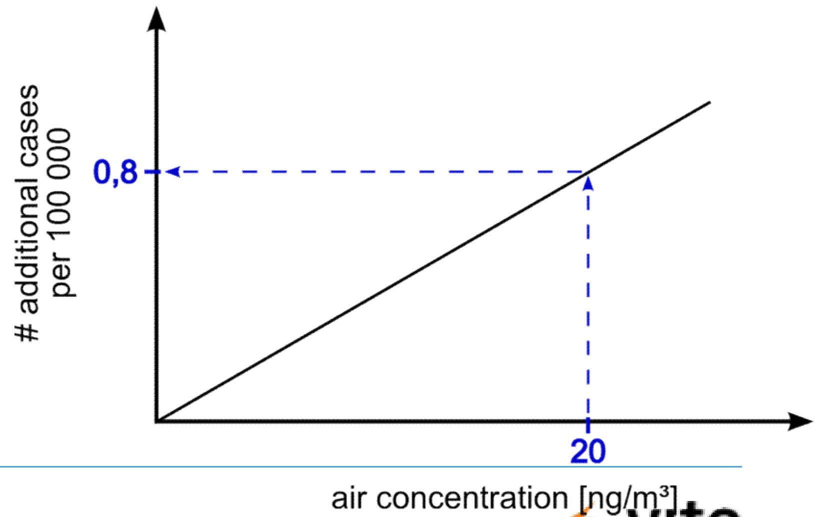
×

$3{,}8 \cdot 10^{-4}$ per µg/m³ (WHO)

=

0,8 additional cases per 100 000

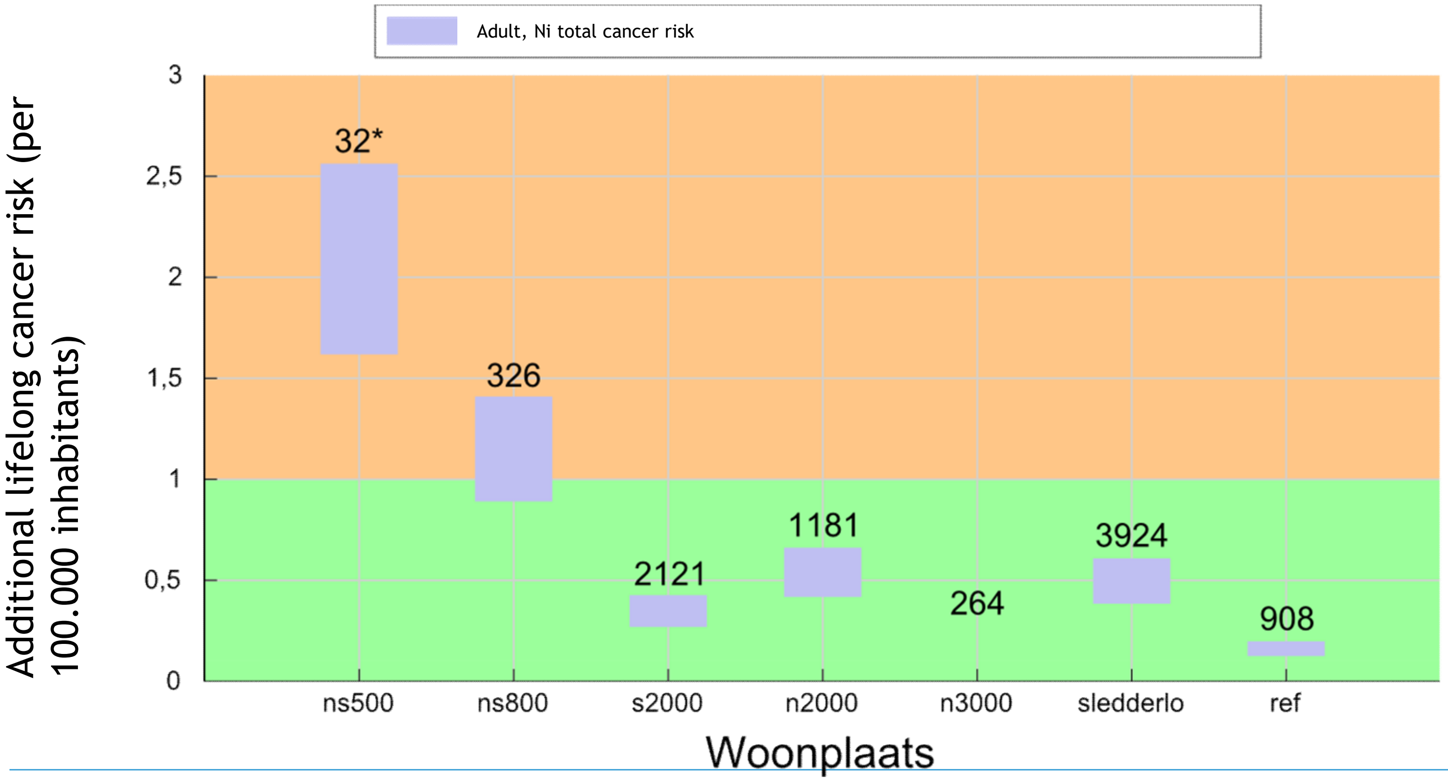
graphical



2. SITE SPECIFIC RISK ASSESSMENT: RESULTS

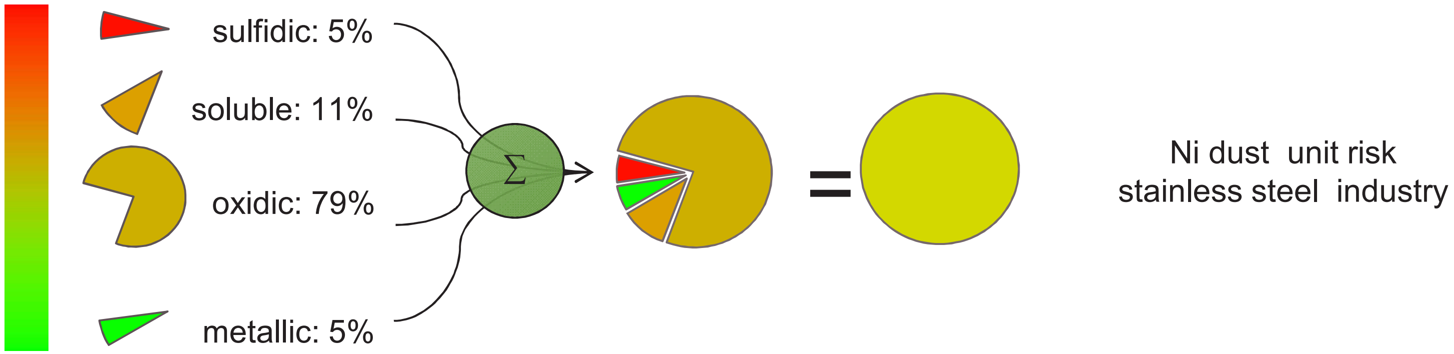
inhalation exposure - carcinogenic effects

*Unit risk **Ni total** : 2.4 10^{-4} per µg/m³ (US EPA) - 3.8 10^{-4} per µg/m³ (WHO)*



2. SITE SPECIFIC RISK ASSESSMENT: RESULTS

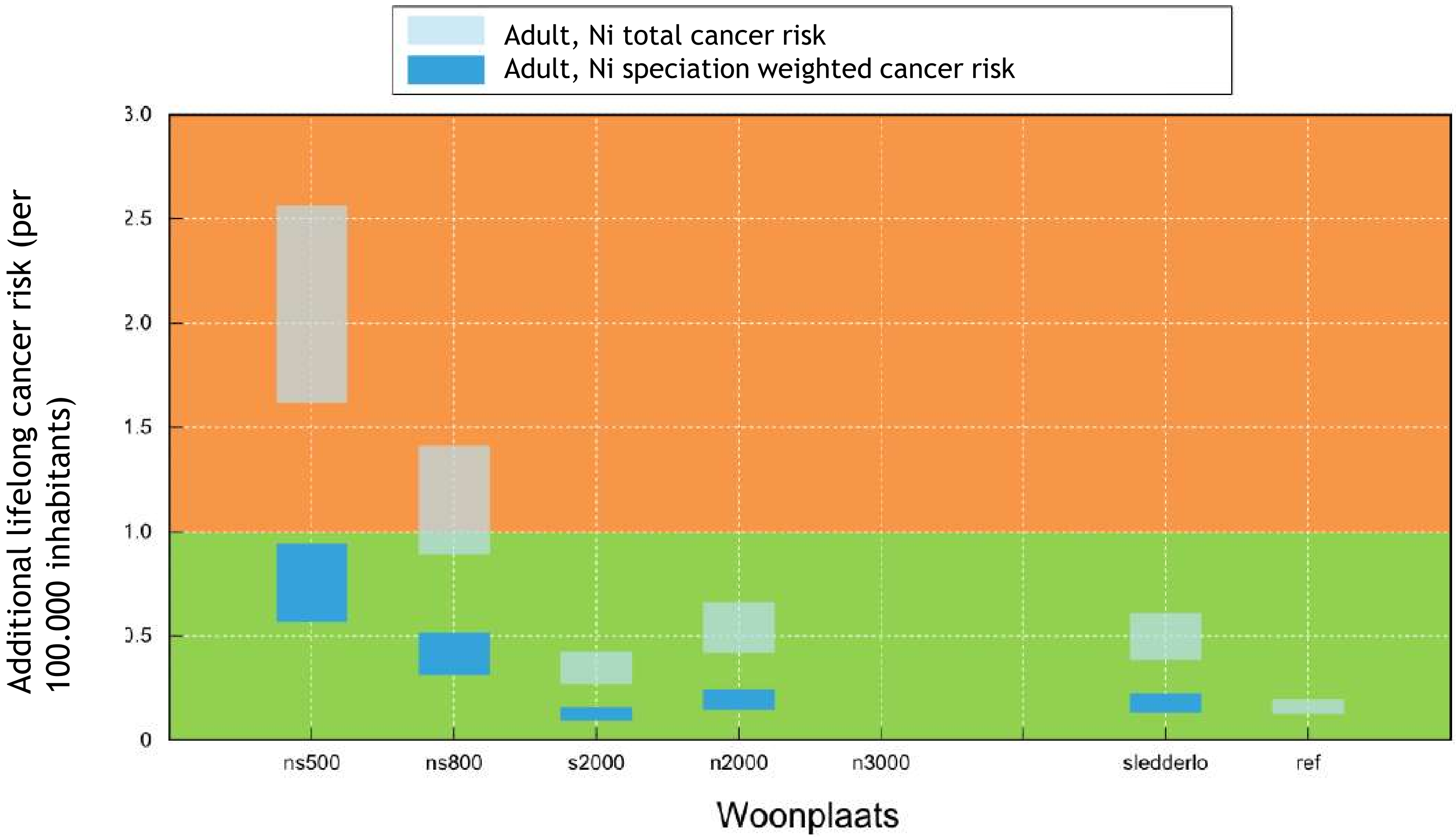
inhalation exposure - carcinogenic effects



Zatka fraction in outdoor air in Sledderlo		***scenario 1***	***scenario 2***	***scenario 3***
		Unit risk ($\mu g/m^3)^{-1}$*	*Unit risk* ($\mu g/m^3)^{-1}$*	*Unit risk* ($\mu g/m^3)^{-1}$*
soluble Ni	*11 %*	$7{,}0 \cdot 10^{-4}$	$3{,}8 \cdot 10^{-4}$	$2{,}4 \cdot 10^{-4}$
oxidic Ni	*79 %*	$4{,}0 \cdot 10^{-5}$	$4{,}0 \cdot 10^{-5}$	$4{,}0 \cdot 10^{-5}$
metallic Ni	*5 %*	-	-	-
sulfidic Ni	*5 %*	$4{,}8 \cdot 10^{-4}$	$4{,}8 \cdot 10^{-4}$	$4{,}8 \cdot 10^{-4}$
Speciation weighted unit risk		$\mathbf{1{,}4 \cdot 10^{-4}}$	$\mathbf{1{,}0 \cdot 10^{-4}}$	$\mathbf{8{,}4 \cdot 10^{-5}}$

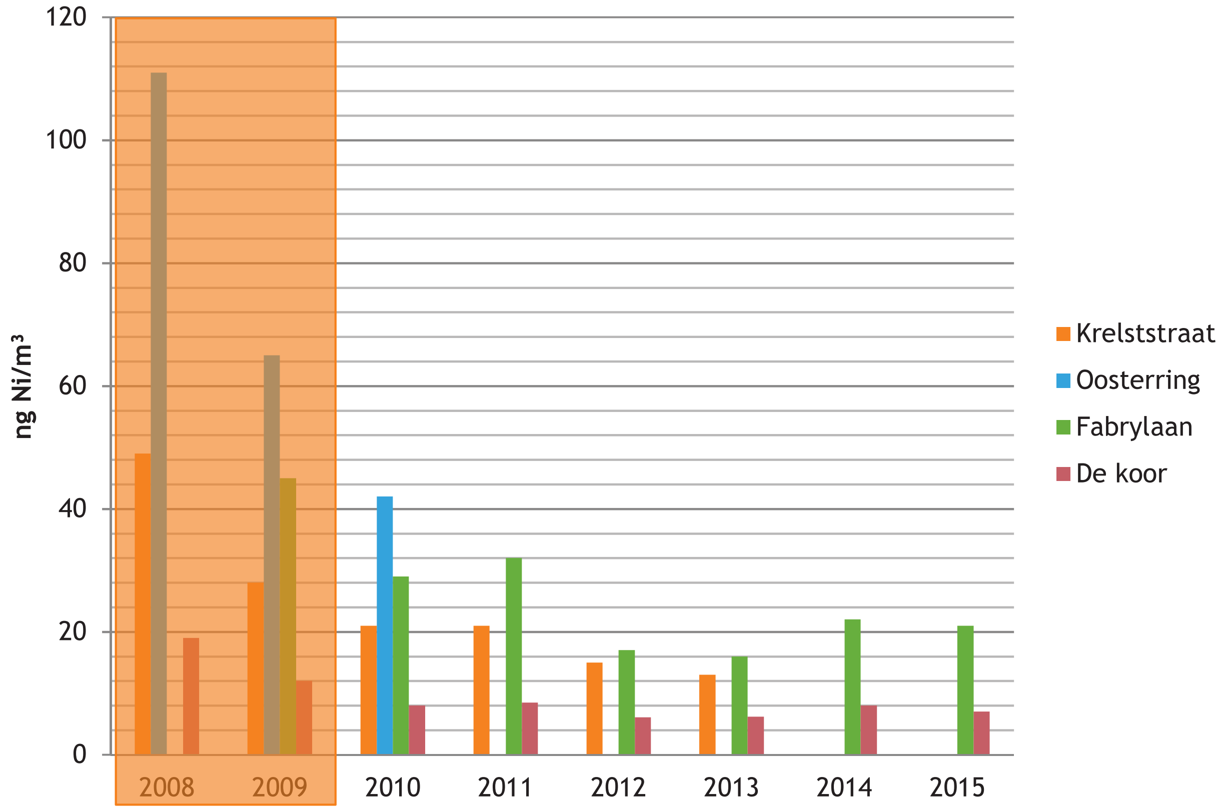
2. SITE SPECIFIC RISK ASSESSMENT: RESULTS

inhalation exposure - carcinogenic effects



2. SITE SPECIFIC RISK ASSESSMENT: OUTLOOK

Numbers based on 2008 – 2009 monitoring data : decreasing trends Ni ambient air around the SS site 2008 – 2015



Take trends into account for lifetime exposure assessment

Context of the study

- Centre for Expertise on Environment and Health
  - Scientific partners:
    - All Flemish universities;
    - 2 research institutes: VITO, PIH
  - Financed, steered and commissioned by the Flemish government:
  - 2007-2011: second cycle of Centre for Expertise on E&H
    - AIMS:
      - Develop Flemish reference values for a large set of pollutants: historical + new emerging chemicals
      - Assess exposure in 2 hot spot areas: Genk-South & Menen

- Outside context of REACH; beyond one industrial plant

3. BIOMONITORING IN GENK – SOUTH

Why Genk South as hotspot?

Industrial zone

- » Industries: stainless steel, car production, chipboard, power station (coal, biomass)
- » High traffic density

Environmental monitoring

- » heavy metals, PCB126, dioxin (dust, soil, vegetables)

Population

- Low SES, high proportion of Turkish, Maroccan immigrants
- Health study (questionnaires) (2007):
  - Complaints: traffic, noise, air pollution, odour
  - Health problems: airway problems, antidepressant medication

3. BIOMONITORING IN GENK – SOUTH

Aim of the study ?

Is living in the neighborhood of Genk-Zuid
- » associated with increased exposure to chemicals?
- » associated with health effects?

HUMAN BIOMONITORING:

"A method for assessing human exposure to chemicals by measuring the chemicals, their metabolites or reaction products in human tissues or specimens, such as blood or urine"

- » 200 adolescents in Genk-Zuid vs. Flemish reference group
- » selection of biomarkers: based in inventory of industry and environmental monitoring
  - → heavy metals, POPs, PAH, benzene, toluene
    + associated health effects

Main findings

Biomonitoring in adolescents of Genk-South pinpoints specific patterns of exposure and biological effects:

» increased exposure to heavy metals : Cd, Cr, Cu, Th, As

» lower levels of Ni, Sb

» increased exposure to PAHs

» lower levels of chlorinated and brominated POPs

» increased DNA damage

» subtle effects on puberty & neurology

Biomarkers of exposure to metals

Biomarker	Genk-South vs. Flanders	p
Blood cadmium	+10%	0.14
Urinary cadmium	+18%	0.008
Blood chromium	+32%	<0.001
Blood copper	+5%	0.009
Urinary copper	+11%	0.03
Blood thallium	+11%	<0.001
Urinary thallium	+8%	0.16
Urin. toxic arsenic	+32%	0.001
Blood manganese	+2%	0.42
Blood lead	-2%	0.63
Blood nickel	-7%	0.03
Urinary nickel	-8%	0.30
Urinary antimony	-21%	0.003

Main findings

Urinary chromium: associated with immissions on 3 days before urine sampling

3-day immission	urinary Cr
20 ng/m^3	0.276 ng/L
100 ng/m^3	0.313 ng/L
200 ng/m^3	0.360 ng/L

Blood lead: associated with distance between domicile and industry

distance	blood lead
500 m	15.1 µg/L
1000 m	14.7 µg/L
2000 m	14.0 µg/L

www.milieu-en-gezondheid.be

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CONCLUDING REMARKS AND OUTLOOK

1. Screening under Ni REACH CSR and site specific assessment:
   » risk from oral Ni exposure < risk from inhalation Ni exposure

2. Opportunities to apply approaches from site specific assessmnent (outside REACH context) → refine critical pathways under REACH MvE CSR and SEA

   » Speciation weighted unit risk approach
   » Accounting for population size
   » Use of monitoring data for 'local scale' assessments in REACH

3. Approach was elaborated for Nickel; consider similar approach for Chromium ?

4. Biomonitoring as a powerful monitoring tool in Man via Environmen Exposure assessment:
   » Measuring human exposure, complementory to forward exposure modelling
   » Outside 'the box' of one industrial plant

3. Modeling aspects and key data sets that may improve the MvE scenario in a tiered way

What key assumptions drive the technical assessment that can be improved through local/regional data gathering and sensitivity assessment

By Volaine Verougstraete and Hugo Waeterschoot,

(Eurometaux)

What key assumptions influence the MvE scenario?

Assume

- WORKPLACE :
  - a "DMEL" around 10^{-4} , 50 workers, 8hs a day and 10 y working experience
- MvE:
  - a "DMEL" around 10^{-6}, 10000 inhabitants, 24hs a day and 70 ys living
- Ambient local exposure (L) 1/100 of workers levels and regional (R) 1/1000

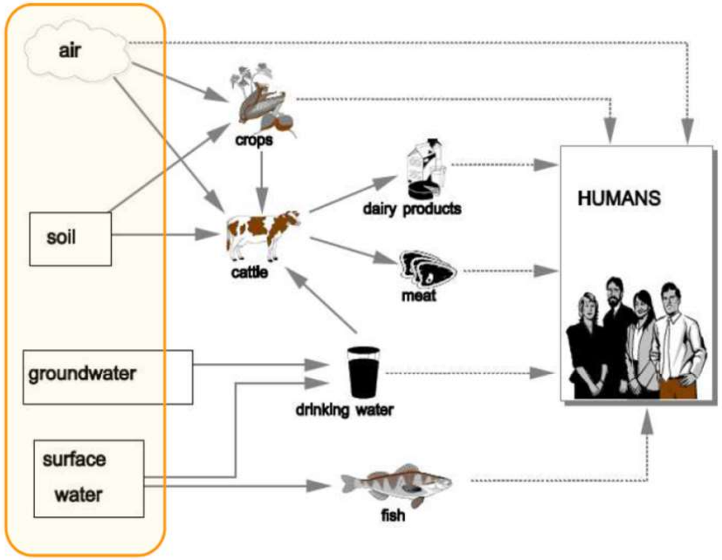
The ~~**MvE is much more sensive because for the RA and the SEA**~~:

Difference in:

- impact: 10^{-4} workers = 10^{-6} local or general population
- exposed population: MvE L: 200 x workers
  MvE R: 20 mio vs 50 !!!
- exposure time: MvE L: (24/8)*(70/20)=10 x more

So in this case the **MvE excess risk >>100 x more SEA impacting scenario than the workplace when only based on estimated inhalation exposure**

What defaults when using: *The modeling concept?*

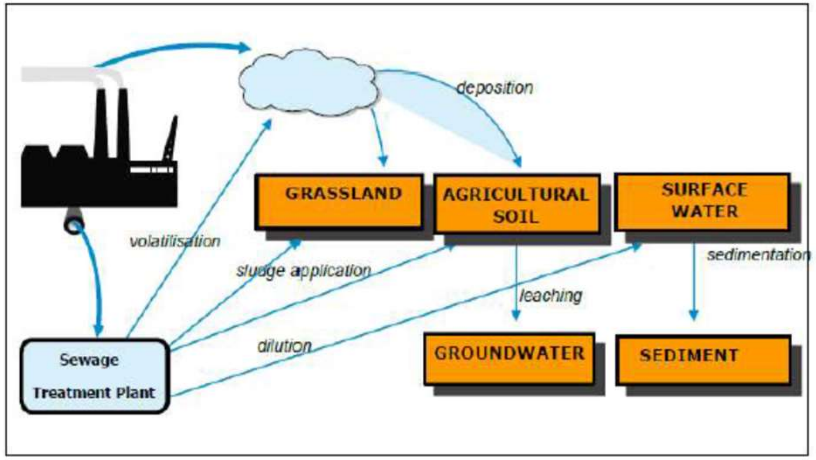


Indirect exposure to humans via the environment

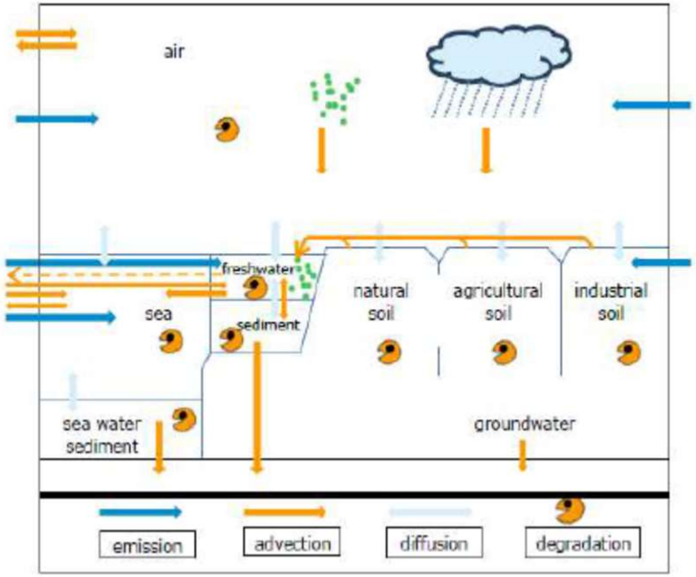
- Default assessment of indirect exposure of humans based on:
  - Estimated inhalation concentration (mg/m³) — **Air modeling**
  - Estimated concentration in food products (mg/kg) — **Food – Drinking water concentration modeling**
    - leaf crops (including cereals and fruit)
    - root crops
    - milk
    - meat
    - fish
    - drinking water
  - Estimated total human doses (mg/kg bw/day) — **Human uptake modeling**
    - Standard inhalation rate and bodyweight assumptions
    - Standard food / water consumption rates

What are conceptual challenges for metals?

Local assessment



Regional assessment



For **RISK ASSESSMENT**

All consumption from local cultivation

- Steady State conditions a
- Scale of the region

For **SOCIO ECONOMIC ASSESSMENT**

- Calculation based on "excess risk"

- multiplied by n° inhabitants !

Why is it a modelling challenge?

The way how:

- The **ambient air levels** are estimated
    - plume modeling at a fixed distance
- **Concentrations in water and soil** are estimated
    - Kp based, sludge from local WWTP
- The way how **intakes are modeled**
    - Biotransfer factors
- The n° of **estimated exposed people**:
    - 10.000 or 20 million inhabitants !
- The "**excess risk basis**"
    - "*any exposure*" contributes to the risk (for non thresholds) even when in the order of background level

Why is it a data gap challenge?

Lots of Defaults used in case of absence of data

A recipe for a problematic assessment for metals

WHEN CRITICAL DATA ARE LACKING

For the EUSES model: substance properties

Parameter	Description	Source
MOLW	Molecular weight	Technical dossier – chapter 1.1
MP	Melting point of substance	Technical dossier– chapter 4
BP	Boiling point of substance	Technical dossier– chapter 4
VP	Vapour pressure of substance	Technical dossier– chap[illegible]8
SOL	Water solubility of substance	Technical dossier– chapter 4
K_{OW}	Octanol water partition coefficient of substance (not relevant for inorganics)	Technical dossier– chapter 4
Biode-gradability	Results of screening test on biodegradability. Not relevant for inorganic substances.	Technical dossier– chapter 5 See also Appendix [illegible].16-3.2

For the ENV. EXPOSURE assessment

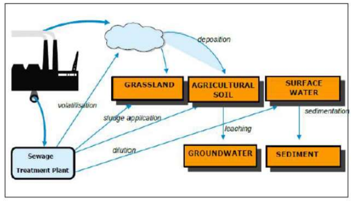
ENVIRONMENTAL CONCENTRATIONS USED AS INPUT FOR INDIRECT EXPOSURE CALCULATIONS		
Compartment	**Local assessment**	**Regional assessment**
surface water	annual average concentration after complete mixing of STP-effluent	steady-state concentration in surface water
air	annual average concentration at 100 m from source or STP (maximum)	steady-state concentration in air
agricultural soil	concentration averaged over 180 days after 10 years of sludge application and aerial deposition	steady-state concentration in agricultural soil
porewater	concentration in porewater of agricultural soil as defined above	steady-state concentration in porewater of agricultural soil
groundwater	concentration in porewater of agricultural soil as defined above	steady-state concentration in porewater of agricultural soil

For the INTAKE assessment

HUMAN DAILY INTAKE OF FOOD AND WATER (FROM EUSES)	
Food	**Intake**
Drinking water	2 l/d
Fish	0.115 kg/d
Leaf crops (incl. fruit and cereals)	1.2 kg/d
Root crops	0.384 kg/d
Meat	0.301 kg/d
Dairy products	0.561 kg/d

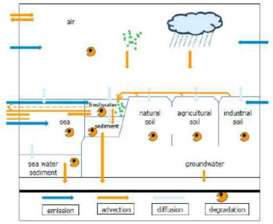
Why can MONITORING even be a challenge?

LOCAL



- Historical pollution impact
- Inhalable versus respirable air
- Household dust exposure
- Relevance of double diet or market basket
- …

REGIONAL



- Seasonal variability in food patterns and exposure patterns
- Inhalable versus respirable
- Contribution via household dust
- Relevance of double diet or market basket dietary studies
- …

What are critical data to improve the assessment?

As a MINIMUM, even this asks for non classical information!

- Know your local town aspects (inhabitants, lifestyle)
- Real exposure data and improved plume modeling
- Is WWTP sludge used

The “real STEP-UP” (= minimum +) but data hungry!

- Ambient values (air-soil-vegetables) and chemical form
- Local gardens/agriculture: how many and what type ?
- Double diet studies for the regional level

Best (=step up +): this is a challenge!

- Local biomonitoring and concentration in food data
- Local disease register

3. Modeling aspects and key data sets that may improve the MvE scenario in a tiered way

Modeling Ambient Air Concentrations of metals at the local scale: tiered approaches and data rquirements

By Wouter Lefebvre, Katleen De Brouwere, Jurgen Buekers
(Vito)

- **Why a tiered approach** (Buekers et al., 2015)?
  - Detailed modelling/monitoring is expensive, has large data requirements, …
  - Therefore, a tiered approach is developed (in this case MvE csr for Ni):
    - In some cases, the emissions are so low that even in worst-case scenario's the DNEL (Derived No Effect Level) will not be reached
    - In other cases, a first (worst-case) guess will exceed the DNEL
      - More detailed study needed
      - Only do monitoring/modelling where needed!

- 1) **C_{total}=$C_{regional}$ + C_{local}**
  - $C_{regional}$ can be determined at a large scale: based on the European AIRBASE dataset for instance.
    - Will be **reasonable worst-case**: as most measurement stations are in high pollution regions
    - For instance: for Ni in Particulate Matter:
      - Countries with at least 15 measurements: Derive mean and P90-value.
      - Apply **P90**/mean-value on all countries
      - Average of all countries: $C_{regional}$
      - For Ni in PM_{10}: 8.5 ng/m³

- 2) RCR = C_{total}/DNEL; lower than 1?

- 3) **Modelling** assumes that emitted substances behave as gases at short distances: ok if substance in fine particulate matter (in PM_{10}), not ok if coarse dust (more deposition); however, tiered approach could be adapted to take that into account.

TIER 1: EUSES model

- **Very simple model** (EUSES 2.0, developed by RIVM)
  - Calculation of local concentration at 100m distance from 1 stack, (stack height 10m, no plume rise), standard Dutch weather conditions
  - Input: Emissions / combination of substance tonnage, release factor, # emission days
  - As stacks are normally higher with plume rise, considered as realistic worst-case assumption
  - As everything is fixed for one stack => based on DNEL you can calculate maximum emission rate for this tier.

TIER 2a: GPM model

- **Simplified Gaussian Plume Model**

(GPM, http://www.arche-consulting.be/Metal-CSA-toolbox/Local-air-modeling-(GPM-tool))

  - Calculation of local concentration at several distances from 100m distance on from 1 stack, standard weather conditions
  - Input: emission rate, wind speed, source height, gas temperature and velocity

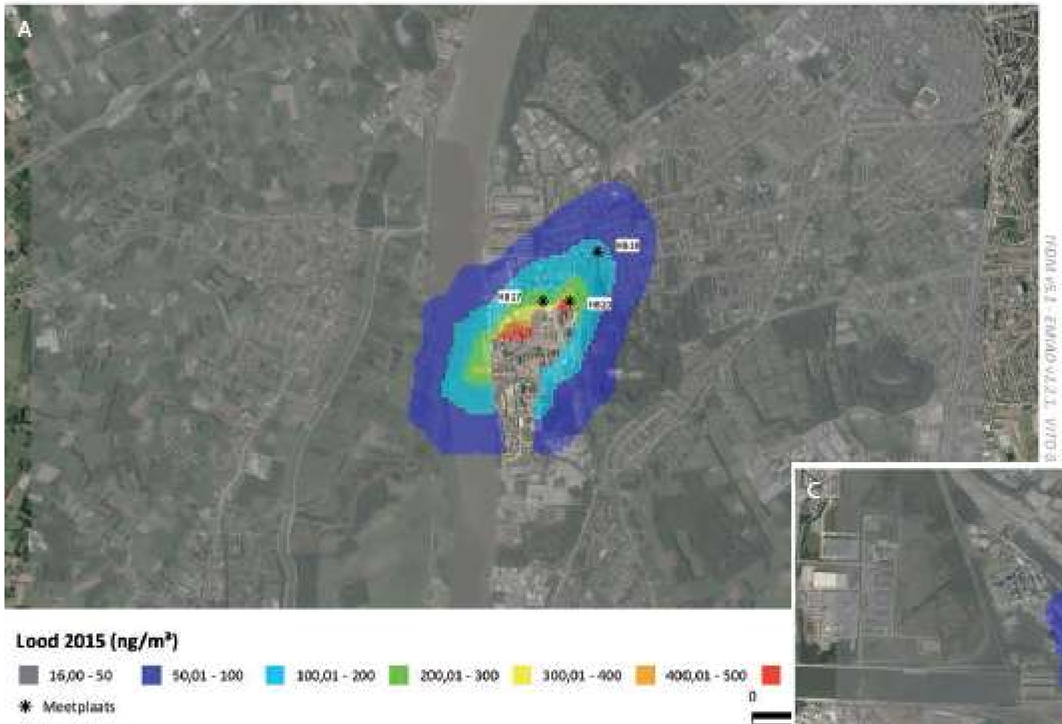
Wind Veloc (m/s)	Estimated Concentration of Ground-Level Pollution (ng/m3) at Selected Distances (km) from Source				
	0,1	0,5	0,8	1,5	3
1	0	0	0	2	34
3	0	1	29	104	95
5	0	11	72	114	74
7	0	23	87	101	58
9	0	31	88	88	47
11	0	35	84	77	40
13	0	37	79	68	34
15	0	37	74	61	30
17	0	37	69	55	27
19	0	36	64	50	24

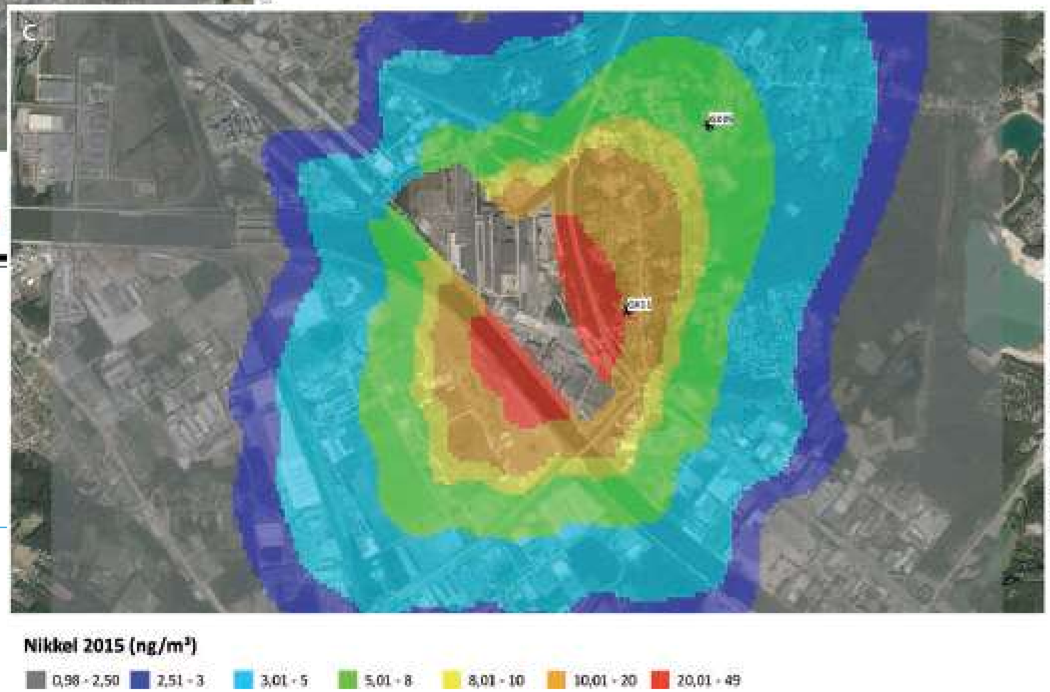
TIER 2b: IFDM model

Complete Gaussian Plume model (IFDM, VITO)

- Calculation of local concentration in a grid around the stacks, multiples stacks, local weather conditions (site-specific, measured, hourly meteorological conditions)
- Input for multiple point sources: locations, emission rates, stack diameters, source height, gas temperature and velocity
- Check not at 100m, but at location where people live!

TIER 2b: IFDM model





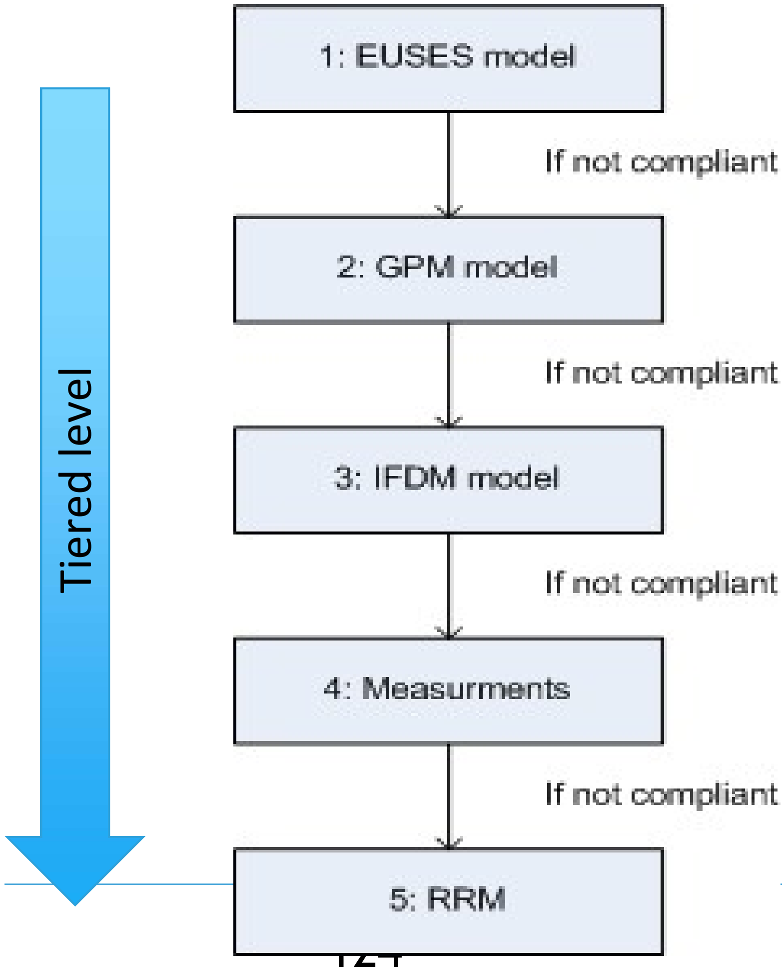
Source: VMM 2016
based on VITO modelling

Tier III: measurements and detailed modelling

- If previous tiers **still give RCR>1:**
  - Monitoring around the site
  - Detailed modelling (including CFD-modelling)

SUMMARY OF TIERED APPROACH

Inhalation exposure



Development of MvE GES from EUSES modelling data:
RCR = 1 at 20 ng/m^3 total
total – background (8.5 ng/m^3) = 11.5 ng/m^3
Recalculate to maximum daily emissions:
<u>41.3 g Ni/day during 365 days</u>

Elaborated for Ni MvE CSR (REACH)

INHALATION EXPOSURE (LOCAL SCALE)

EUSES	GPM	IFDM	monitoring
• Concentration at 100 m distance from point source • Default stack properties • Default, fixed meteorology	• Concentration air along gradient from point source • User – defined stack properties • Default, fixed meteorology	• Concentration air along gradient from point source, time dynamics • User-defined stack properties • Site-specific dynamic meteorological conditions	• Monitoring ambient air (local)

Increased complexity, input requirements and output accuracy →

vito

EXAMPLE

EUSES

PECair, local = 354 ng Ni /m³

At 100 m from point source

+ regional background (8.5 ng/m³)

PECair, local = 362.5 ng Ni /m³

DNEL,local effects = 20 ng/m³

→ RCR = 362.5/20 = 18

→ RCR > 1 → RRM or refine exposure

→ go to GPM model

GPM

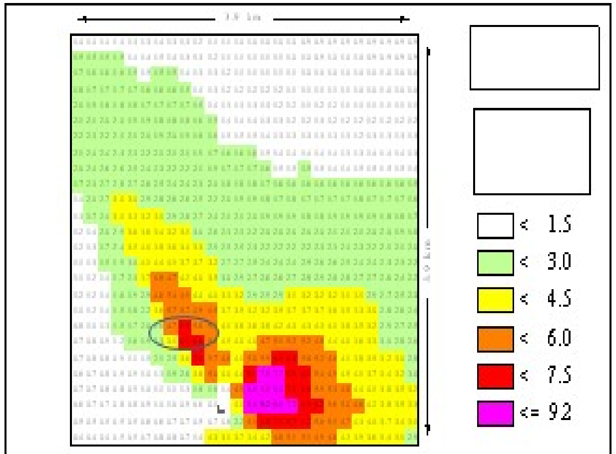
Wind Veloc (m/s)	Estimated Concentration of Ground-Level Pollution (ng/m3) at Selected Distances (km) from Source				
	0,1	0,5	0,8	1,5	3
1	0	0	0	2	34
3	0	1	29	104	95
5	0	11	72	114	74
7	0	23	87	101	58
9	0	31	88	88	47
11	0	35	84	77	40
13	0	37	79	68	34
15	0	37	74	61	30
17	0	37	69	55	27
19	0	36	64	50	24

→ RCR = (114 + 8.5)/20 = 6

→ RCR > 1 → RRM or refine exposure

→ go to IFDM model

IFDM



Gemiddelde (ng/m³) (tav=periode-ge) u

→at distance chosen based on nearest residences

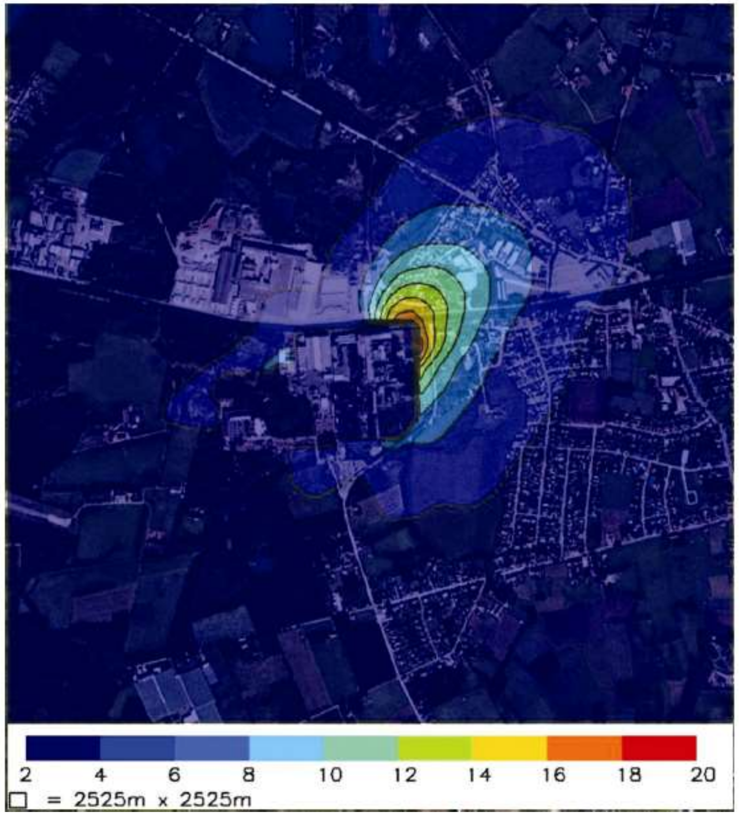
→RCR = (6 + 8.5)/20 = 0.7

→ RCR > 1 → compliance

LIMITATIONS

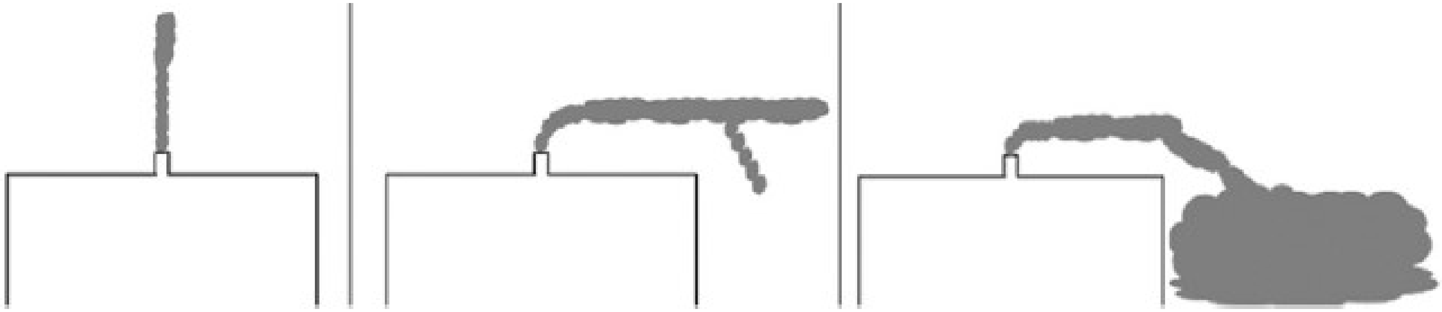
- Not taken into account are diffuse emissions which can be responsible for large part of the concentrations:
  - If estimated: can be included in Tier 2b approach
  - If not estimated: measurements are needed

  - If measurements available: inverse modelling is possible => correct concentration estimates



Source: Lefebvre et al., 2012

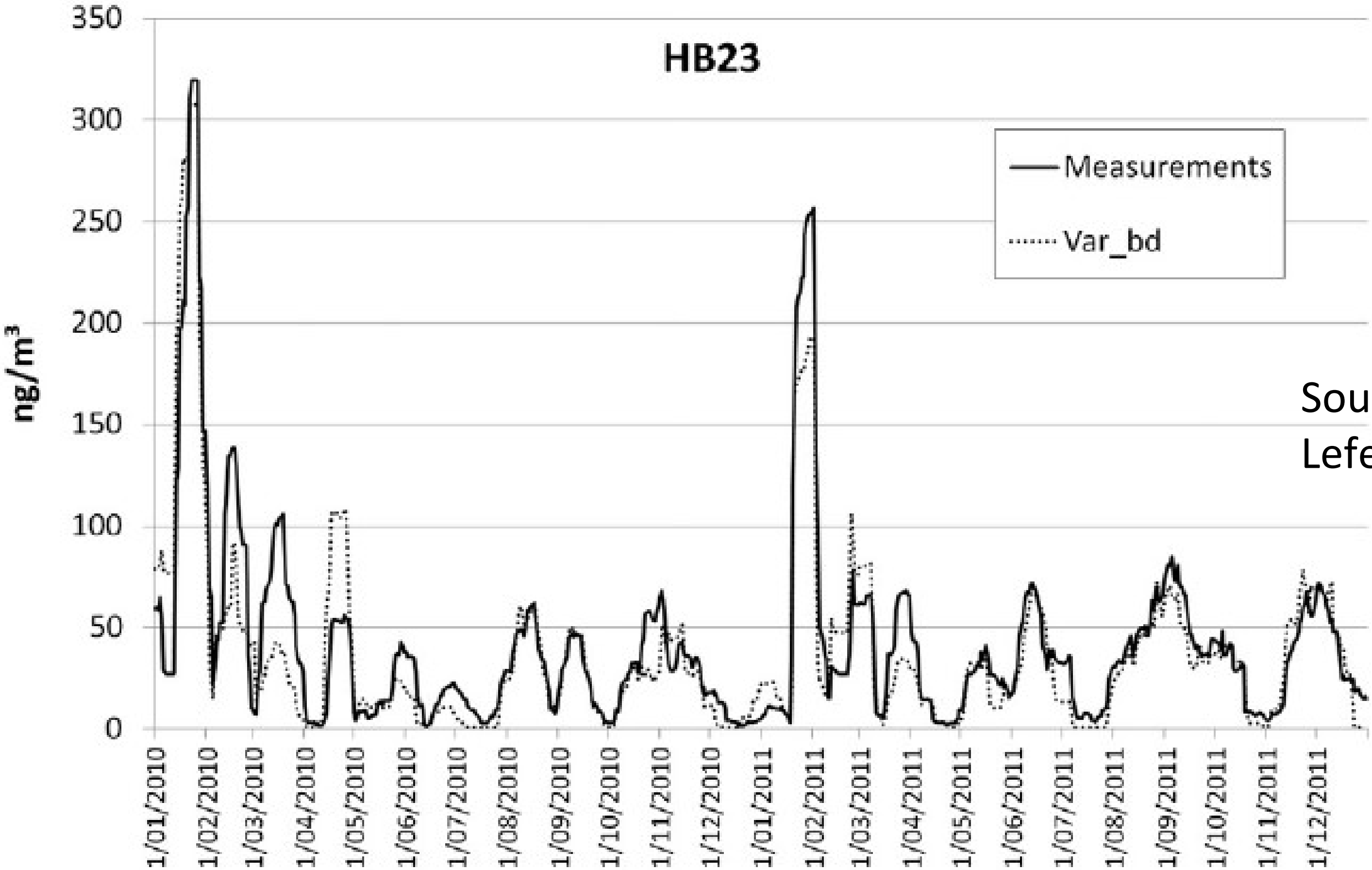
- Building downwash



Needs to be included from Tier2 approach on:

- if applicable (stack height < 2,5 to 3 times building height)
- It is possible to do it: Cosemans et al., 2012; Lefebvre et al., 2013

Building downwash: example of modelling results at site with large building downwash effect



Source:
Lefebvre et al., 2013

- Tiered approach is possible and cost-effective when applied with reason
- Example of application of tiered approach for Ni in air, inhalation pathway: Buekers et al. (2015)
- References:

  - Buekers et al., 2015. Assessment of human exposure to environmental sources of nickel in Europe: inhalation exposure; Science of the Total Environment, 521-522, 359-371.
  - Cosemans et al., 2012. Calculation scheme for a Gaussian parameterization of the Thompson 1991 wind tunnel building downwash dataset, Atm. Env., 59, 355-365.
  - Lefebvre et al., 2013. Comparison of the IFDM building downwash model predictions with field data, Atm. Env., 75, 32-42.
  - Lefebvre et al., 2012. Simulating building downwash of heavy metals by using virtual sources: methodology and results, Int. J. Env. and Pollutions, 48, no. 1/2/3/4, 214-222
  - VMM, 2016. Luchtkwaliteit in het Vlaams Gewest: jaarverslag immissiemeetnetten 2015.

3. Modeling aspects and key data sets that may improve the MvE scenario in a tiered way

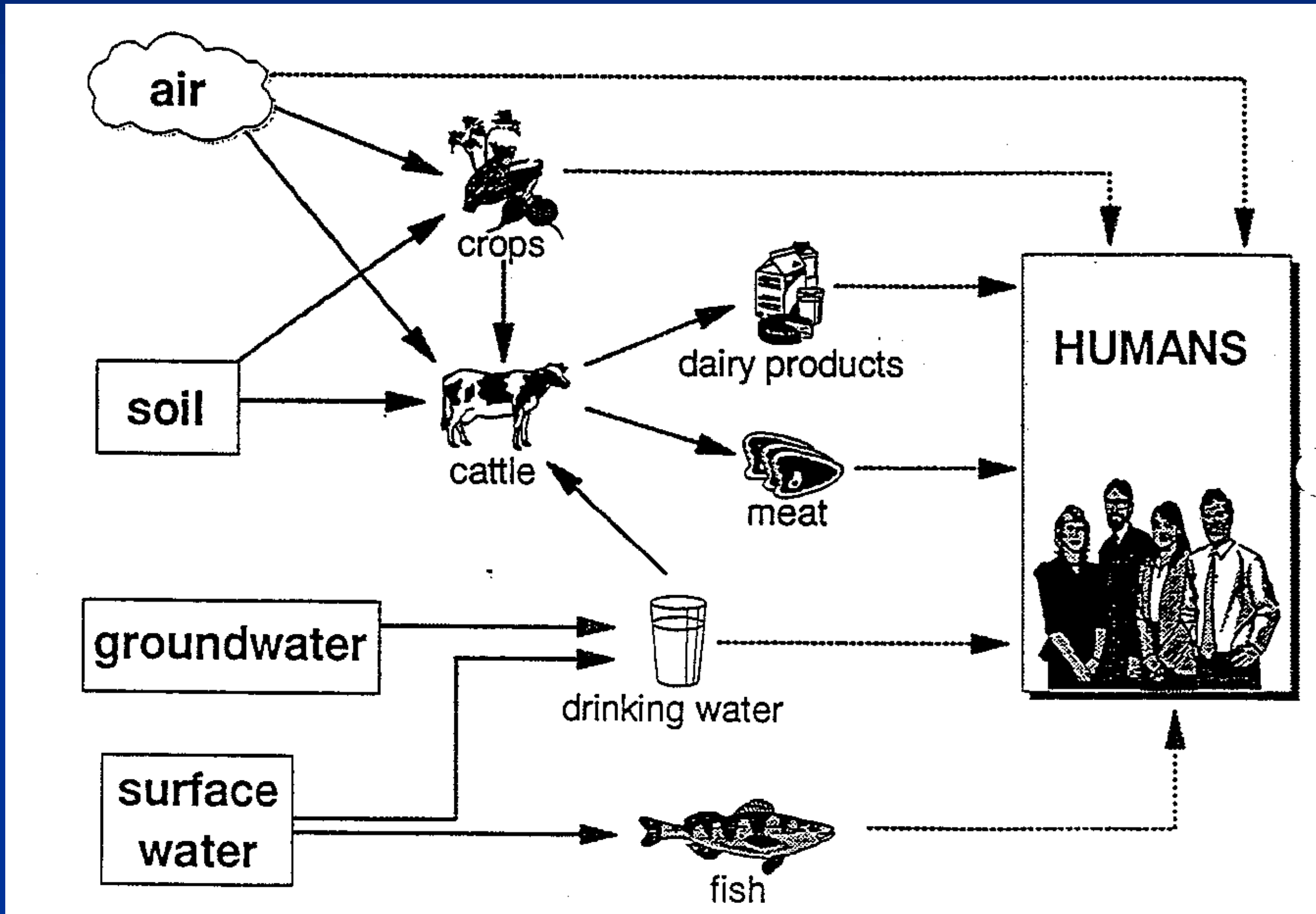
The role and relevance of **Diet Study information**

to improve the Human MvE exposure modeling

By Prof. Erik Smolders,

(KUL)

Exposure of man via the environment



Risk assessment of metals to man are most accurate when based on (biomonitoring) body burden metals, not on environmental metals and its sources

Uncertainty on limits for risk assessment: **High** → **Low**

Fertilisers → Soil → Crops / Food items → Diet → Body burden (kidney)

Uncertainty in asociation related to	other Cd sources	bioavailability	dietary preferences	nutritional status other Cd sources

Example: Cd

Limits	Cd-sludge Cd-phosphate fertilises	SSV	food limits (CODEX)	PTWI PTDI	U-Cd NOAEL

Biomonitoring indicates no risk of Cd in the general, non smoking population in EU while dietary intake data suggest risk, despite equal threshold used to convert body burden to acceptable daily intake

Index	value (95%CI)	threshold	risk?
U-Cd (µg/g cr) P95, 50 y, M&F	0.53 (0.22-0.84)	1.0	no
D-Cd (µg/day) mean, 40y	15.3 (13.9-16.6)	25	no
D-Cd (µg/day) P95	36.6 (EFSA data)	25	yes
D-Cd (µg/kg BW/week) Young adol, 12y	2.7 (2.4-2.9)	2.5	yes

Modelling dietary intake of contaminants

	accuracy
Market Basket (MB)	least
Total Diet Study (TDS)	
Duplicate Meal (D)	
Faecal Excretion (FE)	most

Total Diet Study and Market Basket

Dietary intake of metal (D-M) =

Σ Metal concentration in food item x consumption of food item

= occurence x consumption

Example 1

Cadmium in the Belgian general population *(Vromman et al. 2010, Food Addit Contam)*

(a) occurence….

Food	Number sample	Nb <LOQ	Percent of sample <LOQ	Min ($mg\,kg^{-1}$)	Max ($mg\,kg^{-1}$)	Mean ($mg\,kg^{-1}$)	P50 ($mg\,kg^{-1}$)
Bread	40	1	3	0.005	0.051	0.019	0.019
Pasta, noodle	38	0	0	0.011	0.130	0.060	0.054
Cereals (wheat)	10	0	0	0.025	0.099	0.051	0.052
Potatoes	88	21	24	0.005	0.140	0.023	0.021
Garlic	7	3	43	0.005	0.048	0.014	0.011
Courgette	7	5	71	0.005	0.047	0.012	0.005

(b) consumption and D-Cd

Table 2. Estimation of Cd dietary exposure by the Belgian adult population (>15 year).

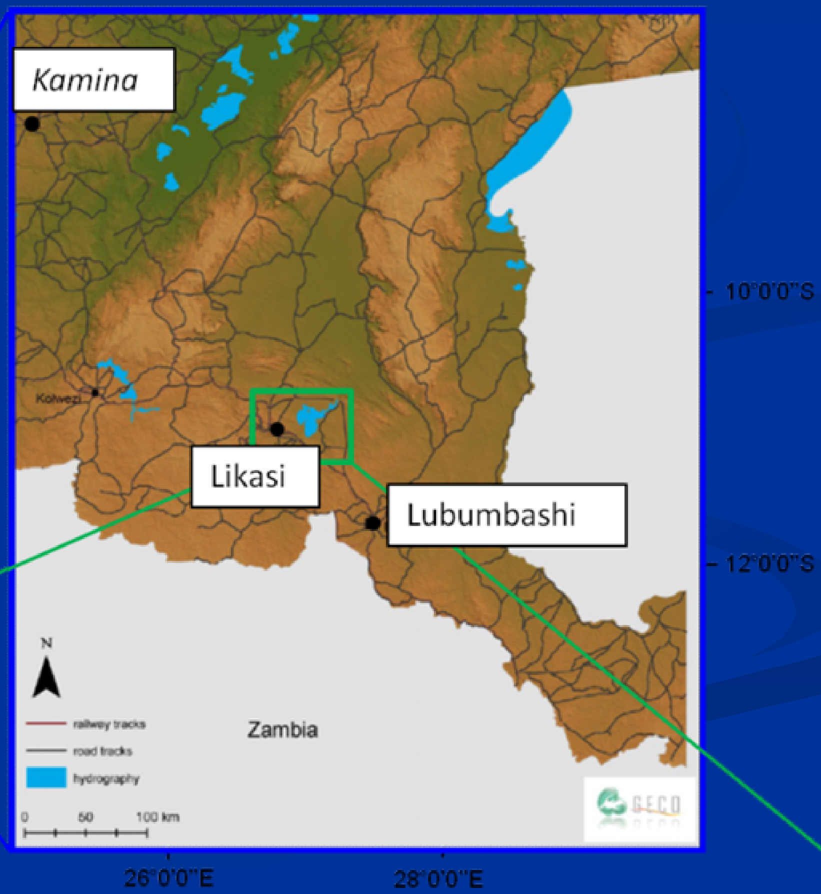
Food	Mean consumption ($kg\,kg^{-1}$ body weight per day)	Exposure ($\mu g\,kg^{-1}$ body weight per week)	%TWI (=2.5 $\mu g\,kg^{-1}$ body weight per week)
Bread	1.75E-03	0.233	9.31
Pasta, noodle	4.66E-04	0.176	7.05
Cereals (wheat)	3.70E-06	0.001	0.05
Potatoes	1.57E-03	0.226	9.03
Garlic	2.58E-06	0.0002	0.01

Contribution of food categories

Table 3. Contribution of food categories to the dietary exposure of the Belgian adult population.

Categories of food	Contribution to exposure (%)
Cereals (wheat), bread	23.83
Potatoes	22.99
Pasta, noodle	17.94
Vegetables	11.34
Beverages (water, juice)	4.80
Meat (poultry, bovine, pork, horse, game)	4.57
Fish	4.47
Crustaceans, bivalves	4.01
Chocolate	3.58
Dairy products	0.97
Fruit	0.82
Offal (horse, game, bovine)	0.57
Eggs	0.05
Honey	0.03

Example 2: exposure of the general population in Katanga to Co



Biomonitoring in the general population of Katanga: urine spot samples, cobalt data

Reference according to NHANES	Control area	Residential area 3-10 km from mining area	Residential area <3 km from mining and refinement	Occupational limit according to ACGIH
U-Co (µg/g creatinine), geomean (P25-P75)				
0.4	1.3 (0.7-2.2)	5.7 (3.2-9.1)	15.7 (5.3-43.2)	15
			87% of children >15 µg/g	

Banza et al., 2009, Environ. Res.

Objectives

Identify cobalt exposure pathways to the general population, i.e. dust, cereals, vegetables, water and fish

Design

Paired sampling of urine (n=253), food items (n=394), soil&dust (n=85) and food questionnaires (n=29)

D-Co estimated as Market Basket approach

Aggregation at household levell (n=29) in locations (n=11) grouped in three regions: polluted, lakeside and control

Cheyns et al. 2014, Sci. Tot. Environ

(a) Consumption

Average estimated consumption for adults (g dry weight/day or mL/day; standard deviations in brackets)

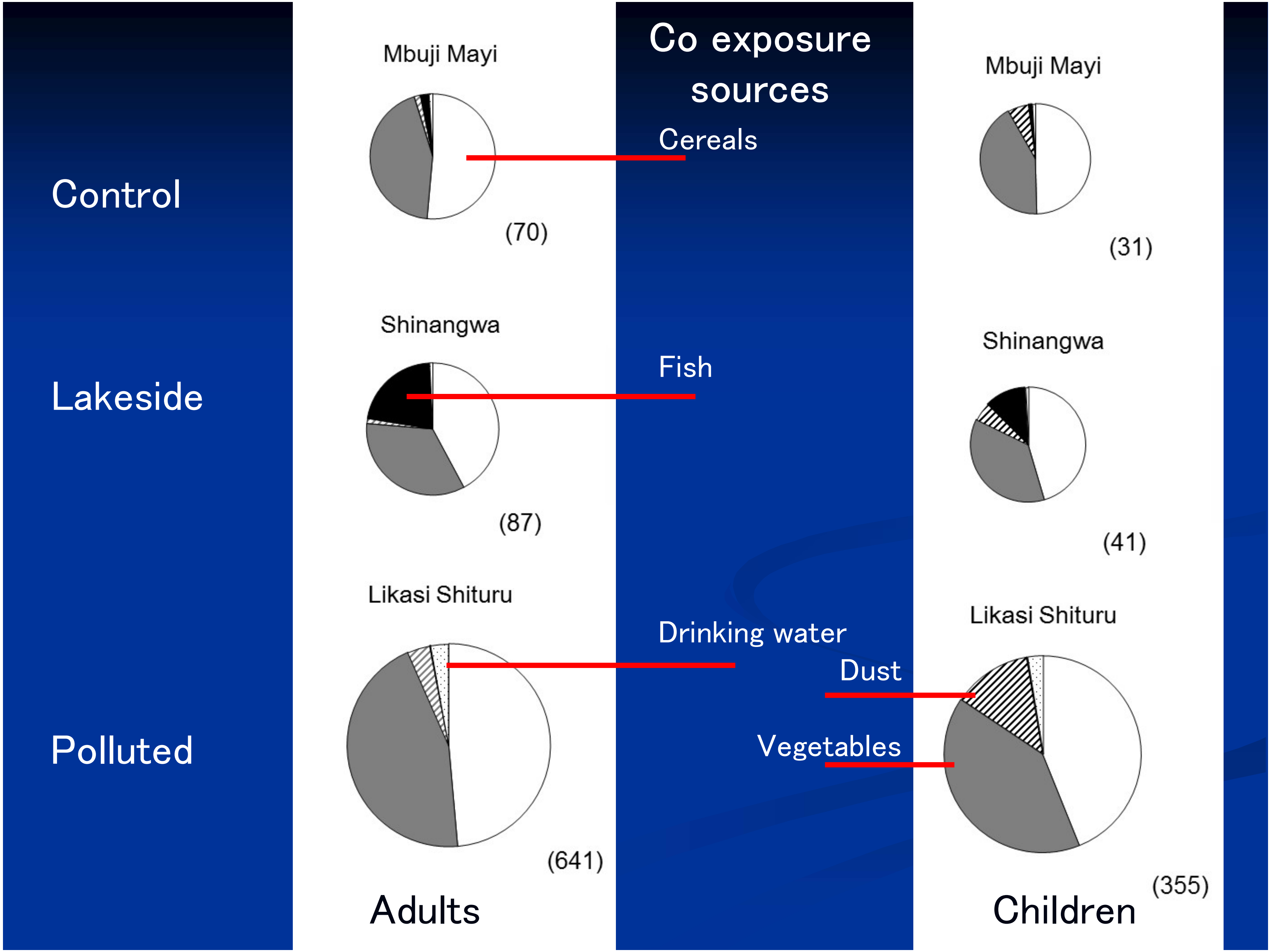
	control area n=5	lakeside area n=9	polluted area n=15
cereals (g/day)	610 (50)	620 (26)	610 (47)
vegetables (g/day)	25 (11)	28 (14)	23 (17)
meat (g/day)	0.6 (11)	0.1 (0.2)	0.5 (0.5)
water (mL/day)	1500 (500)	1500 (500)	1500 (500)
dust$ (g/day)	0.1 (0.05)	0.1 (0.05)	0.1 (0.05)
fish (g/day)	4.1 (1.0)	3.1 (0.8)	2.5 (1.6)

$0.2 g/ for children; assumption, see discussion

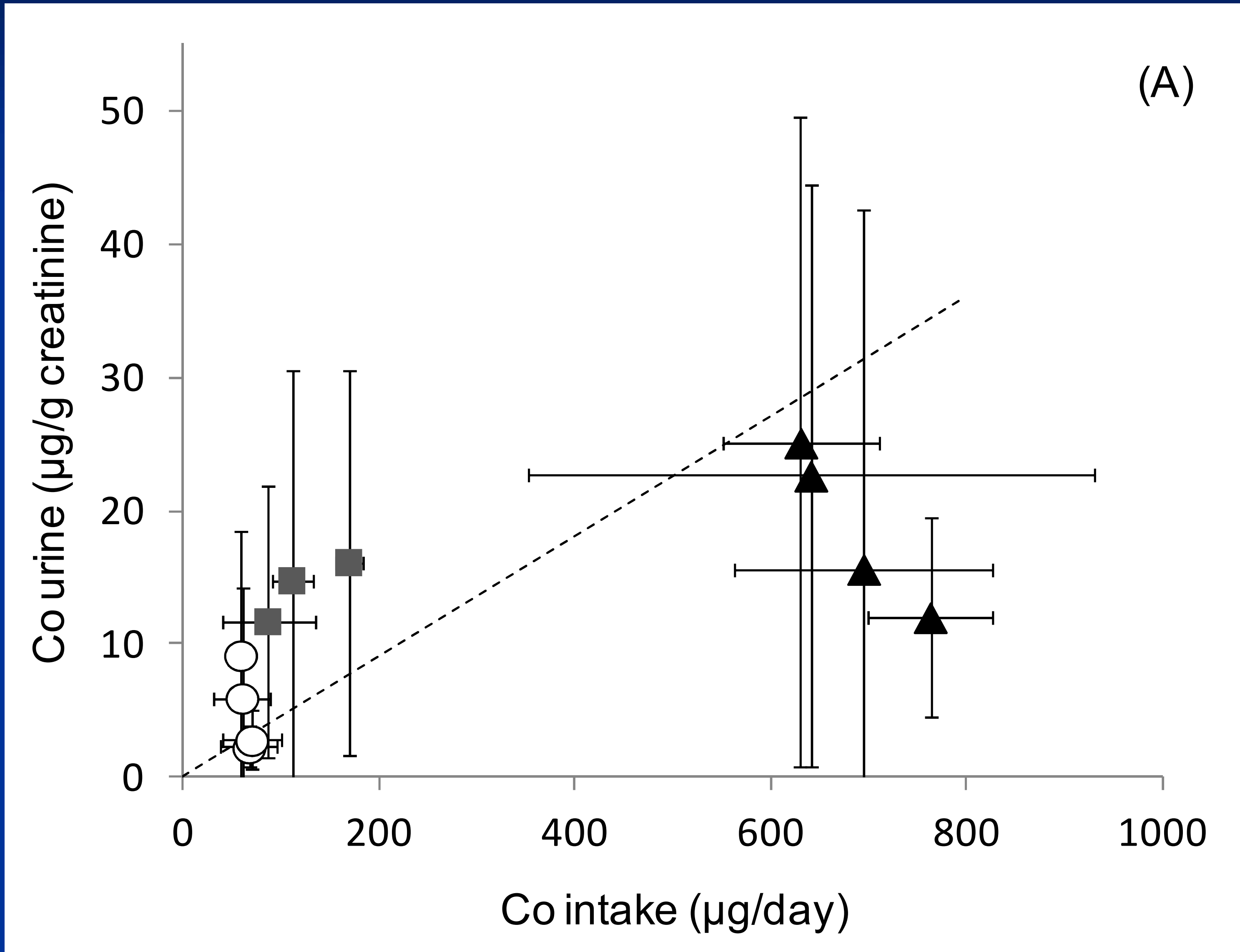
(b) Occurence and D-Co

Average cobalt concentrations (µg Co/g oven dry weight) in environmental samples (n=394); selected data only

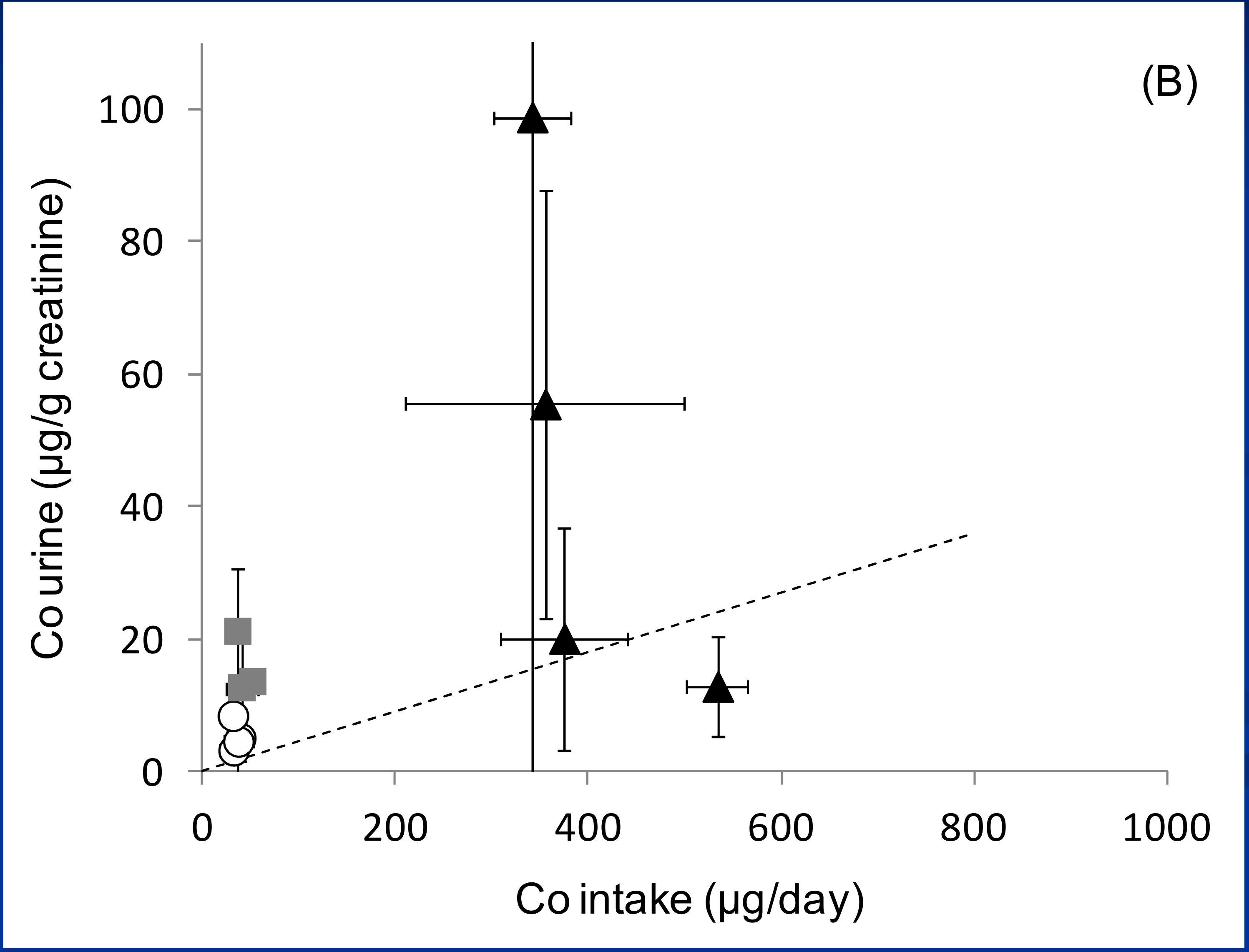
	control + lakeside area		polluted	effect[$$]
maize flour	0.05		0.40	**
tubers	0.21		2.6	**
sweat potato leaves	1.1		6.7	***
leafy vegetables	1.2		46	***
beans	0.84		22	***
drinking water (µg/L)	<0.001		0.012	*
indoor dust	11		440	***
soil	20		132	**
	control	lakeside	polluted	
fish	0.34	6.2	-	***
daily Co intake (µg Co/day), adults	64	120	680	***


Co exposure sources
Control
Lakeside
Polluted
Mbuji Mayi
(70)
Shinangwa
(87)
Likasi Shituru
(641)
Adults
Cereals
Fish
Drinking water
Dust
Vegetables
Mbuji Mayi
(31)
Shinangwa
(41)
Likasi Shituru
(355)
Children

Urine Co in adults related to estimated daily Co intake Means and SD of households per location. Dashed lines: toxicokinetic model of Barceloux, 1999)



Urine Co in children related to estimated daily Co intake Means and SD of households per location. Dashed lines: toxicokinetic model of Barceloux, 1999)



Problems with TDS and MB

1. Aggregation in too limited food categories
2. Consumption: account for variability among individuals and season
3. Occurence: account for variability, LOQ issues
4. The caveat is the estimate of the P95

Food	Number sample	Nb <LOQ	Percent of sample <LOQ	Min (mg kg^{-1})	Max (mg kg^{-1})	Mean (mg kg^{-1})	P50 (mg kg^{-1})
Bread	40	1	3	0.005	0.051	0.019	0.019
Pasta, noodle	38	0	0	0.011	0.130	0.060	0.054
Cereals (wheat)	10	0	0	0.025	0.099	0.051	0.052
Potatoes	88	21	24	0.005	0.140	0.023	0.021
Garlic	7	3	43	0.005	0.048	0.014	0.011
Courgette	7	5	71	0.005	0.047	0.012	0.005
Horse meat	70	8	11	0.005	0.36	0.042	0.031
Horse liver	20	0	0	0.028	72.6	5.315	1.64
Horse kidney	15	0	0	4.430	71.7	19.463	14.7
Game meat	268	245	91	0.005	0.029	0.006	0.005
Game liver	46	0	0	0.015	52.27	2.341	0.17
Game kidney	37	0	0	0.2	14.47	2.768	1.63
Fruit juice	56	54	96	0.005	0.016	0.005	0.005
Mineral water (FAL,** 2000–2003)	14	0	0	0.00005	0.0003	0.0002	0.0002
Chocolate	10	5	50	0.010	0.090	0.034	0.025

Note: *Waegeneers et al. personal communication; **Institute of Plant Nutrition and Soil Science, Federal Agricultural Research Center (FAL) Braunschweig (2000–2003).

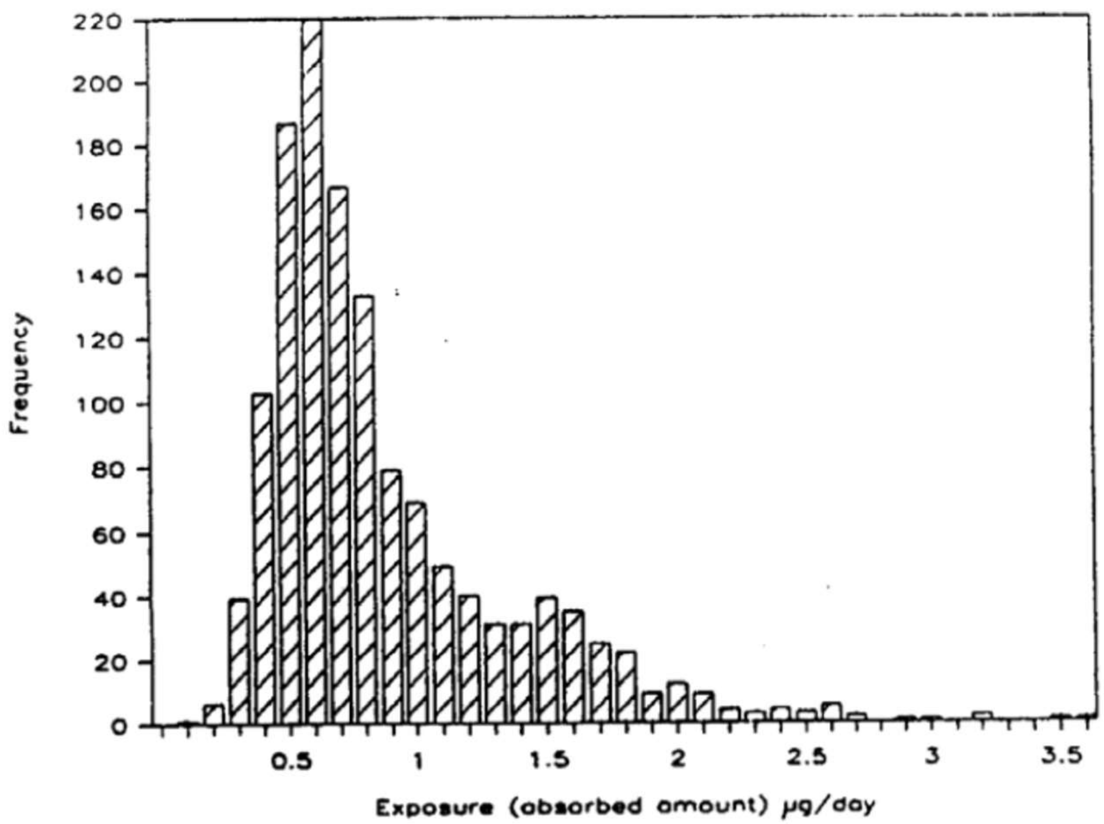
The P95 values in D-Cd are used in risk assessment but there is no standard accurate method.

Methods include:
(a) a P95 based on variance in consumption data using mean occurence
(b) a P95 based on the variance in occurrence data using mean consumption
(c) a mixture of both, often calculated with a probabilistic way (Monte Carlo simulation with random samplings from both distribution).

P95 are also unsure due to the effect of outliers in analytical data and the effect of outliers in consumption data.

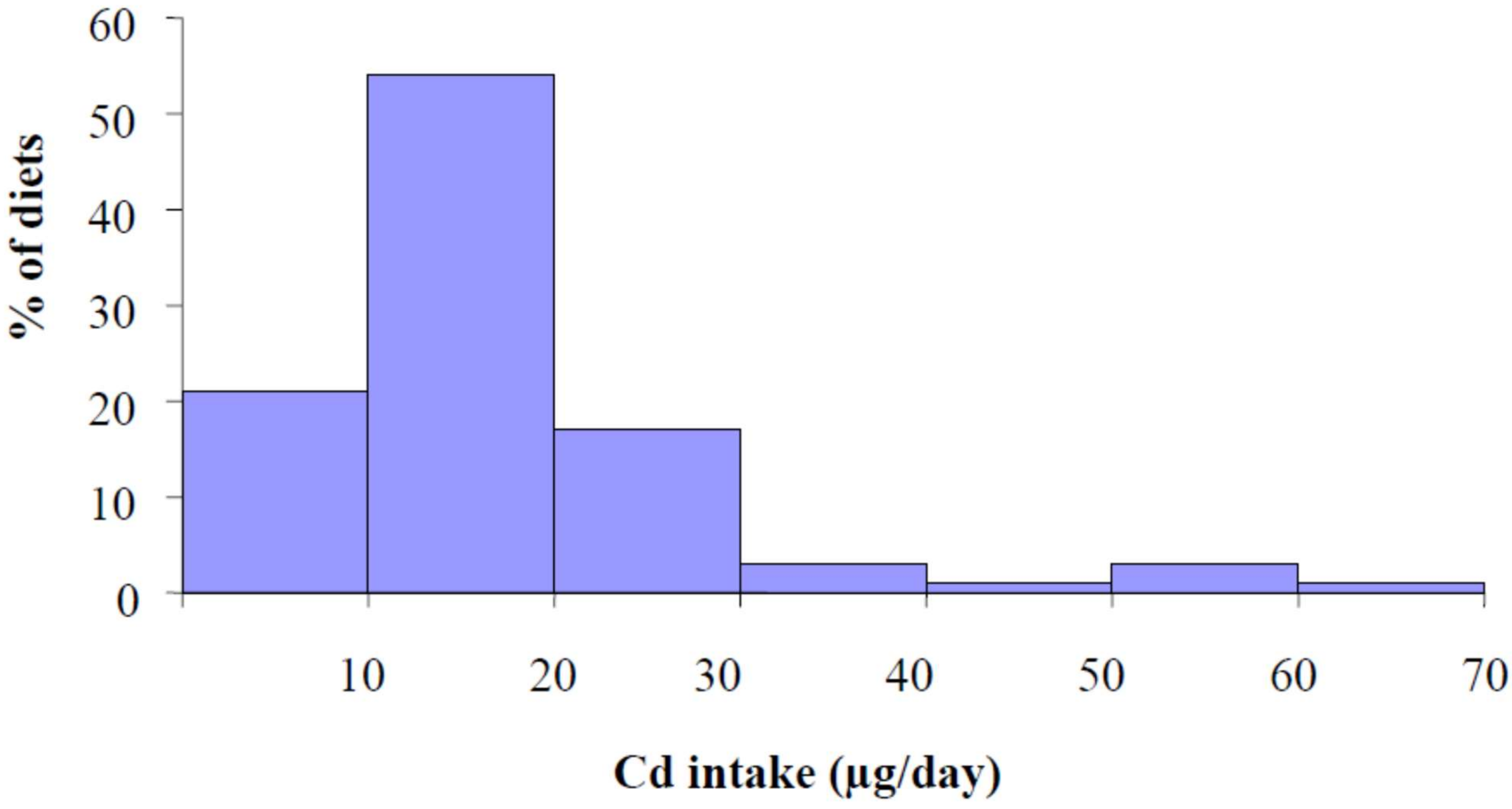
Example of estimating variability among individuals witjh method (a), i.e. using mean occurence data

Figure 4.2 Distribution of Cd exposure to 1348 adult individuals in Finland (25-64 years). The Cd exposure includes intake from food (with 5% absorption from dietary Cd) and smoking habits (0.05 µg Cd absorption per cigarette). Redrawn from Louekari et al. (1989)



Duplicate meal study: accounts for true variance in intake

Figure 4.1 The frequency distribution of duplicate diets, collected during 4 consecutive days, of 74 Swedish women (20-50 years
Redrawn after Berglund et al. (1994) and Vahter et al. (1996)



Duplicate meal and fecal excretion study agree (Vahter et al., 1996)

TABLE 2

Cadmium in Daily Duplicate Diets (Average of 4 Consecutive Days) and Corresponding Feces in Relation to the Type of Diet

	Mixed diet (n = 34)	Shellfish (n = 17)
Cd in duplicate diets, μg/day		
Mean (SD)	11.1 (4.2)	27.8 (17.6)
Median	10.5	22.3
Range[a]	5.7–25.8	9.0–70.0
Range all Diets[b]	2.0–46.8	3.2–175
		$p < 0.0001$
Fecal Cd, % of diet Cd[c]		
Mean (SD)	98.0 (7.9)	101.0 (5.8)
Median	98.9	100
Range[a]	75.4–113	92.9–121

[a] Range of average daily dietary/fecal Cd content among the women.

[b] Range of Cd content in all collected daily diets. N = 136 in mixed diet group, N = 68 in shellfish group.

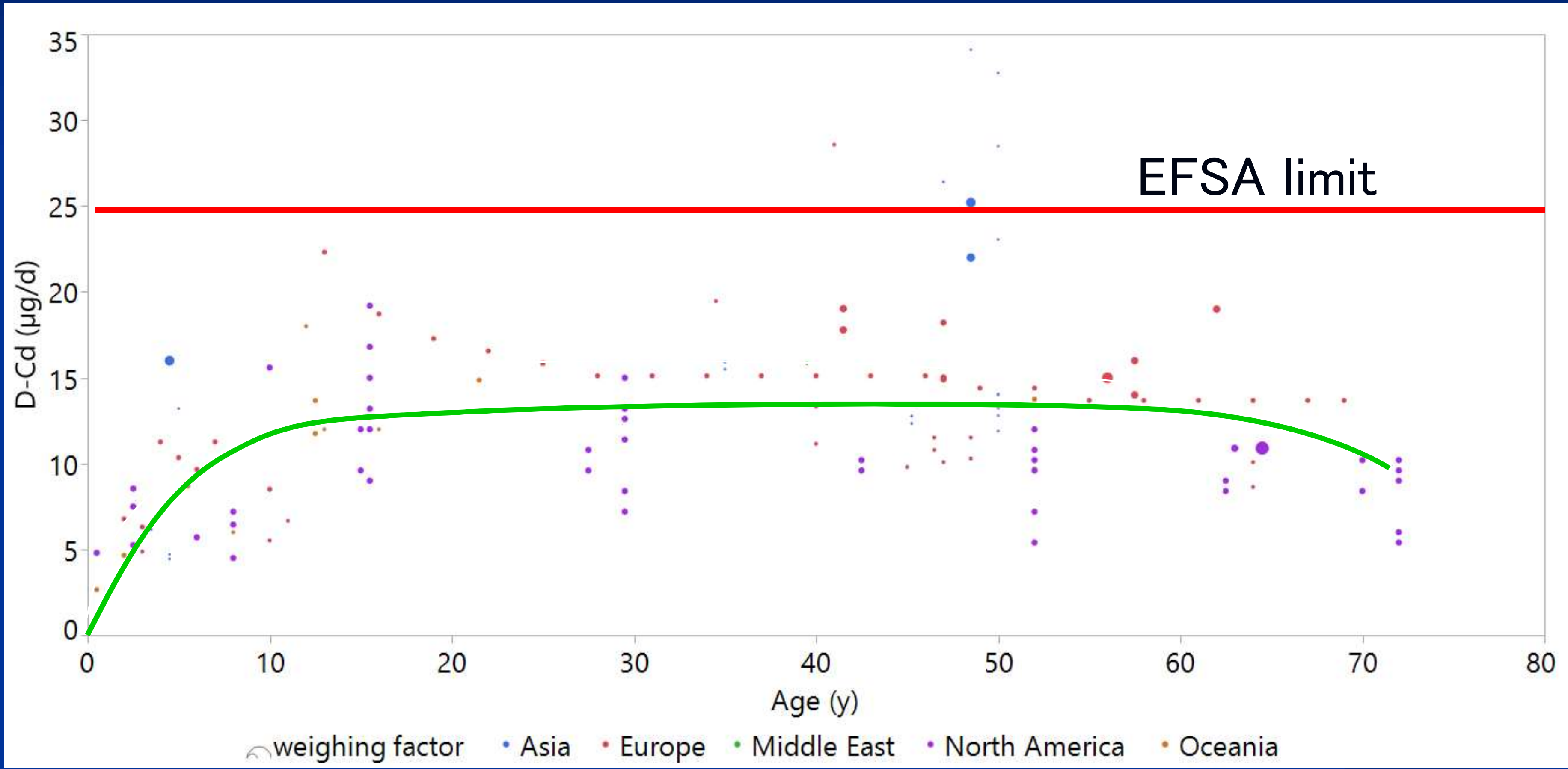
[c] Total fecal Cd between colored markers in % of total dietary Cd during the 4-day study period.

Expression of dietary dose:

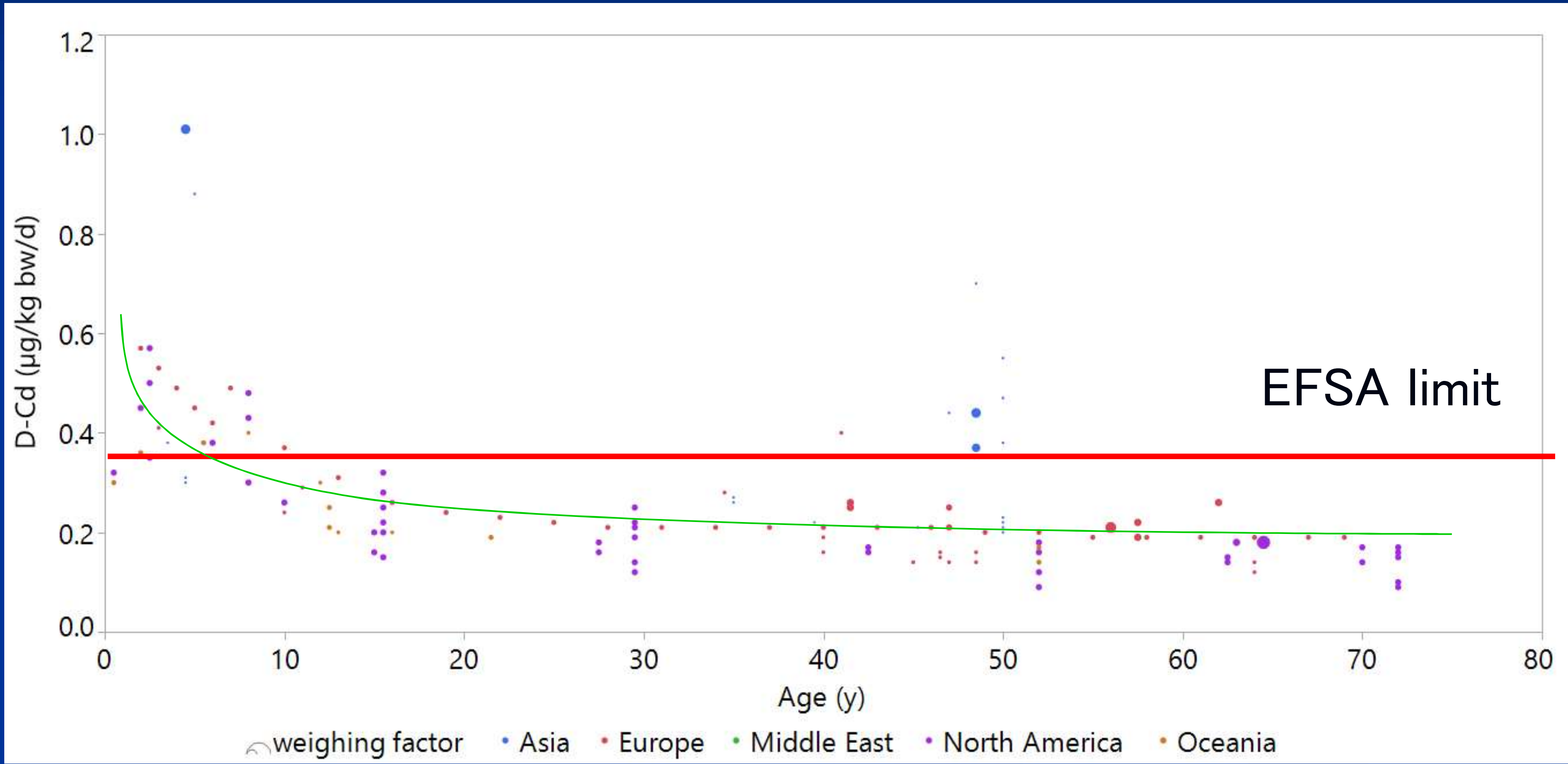
Body weight corrected or not?

Worldwide compilation

Daily Cd intake expressed as µg Cd/day



Worldwide compilation:
Daily Cd intake expressed as µg Cd/kg body weight/day



…and so, using body weight corrected assessments led to the Cd in cacao limits in Europe

which indicates a statistical significant but marginal exposure

consumption ($n = 111$; $p = 0.01$; Table 1). Children reporting a high consumption of chocolate (several times per week) had higher gm UCd (0.067 µg/g crea; $n = 1050$) than those reporting a lower consumption (0.062 µg/g crea; $n = 634$; $p = 0.03$), while children

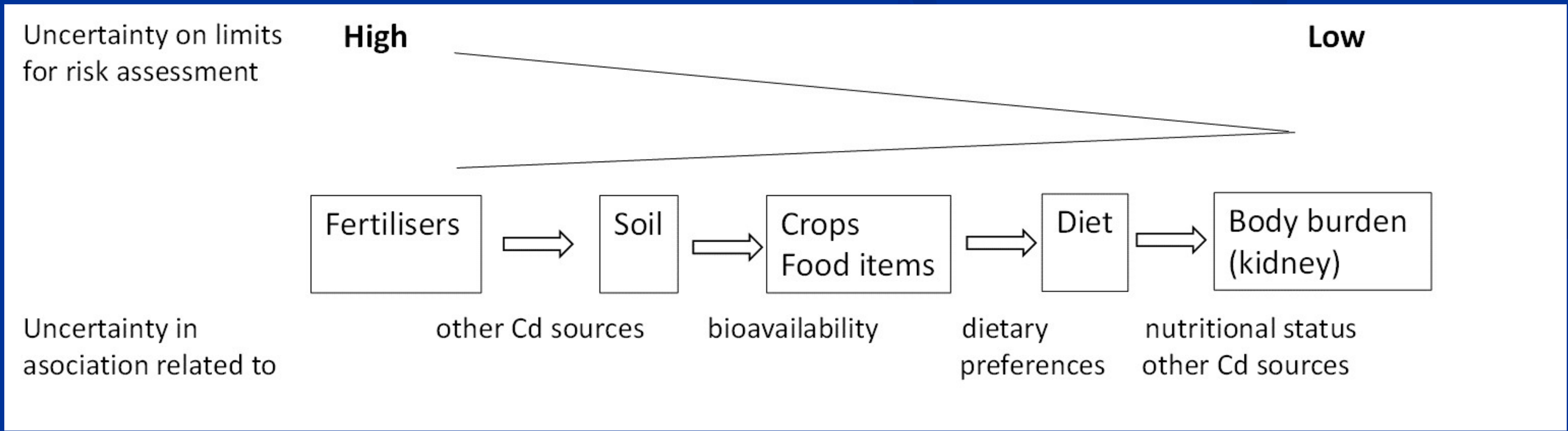
Berglund et al., 2015

Dust ingestion: a critical aspect･･･sometimes


MEICHENG

Conclusion

- Dietary metal (D-M) intake is an index of exposure but risk assessment requires careful attention to the conversion to body burden and, hence, true exposure
- The identification of upper percentiles of D-M is preferably based on duplicate meal of fecal excretion studies that are more accurate than market basket studies



3. Modeling aspects and key data sets that may improve the MvE scenario in a tiered way

Alternative modeling options for integrated MvE exposure at the regional and local scale: development of a tiered appraoch for metals in the **MERLIN-expo tool**

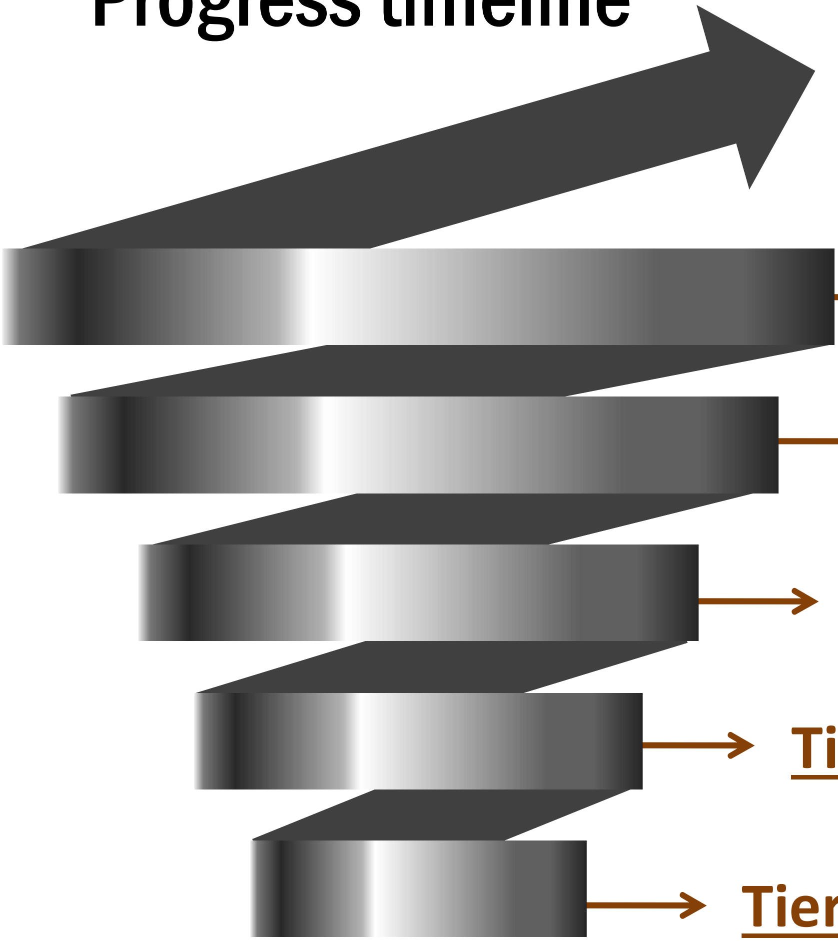
By Katleen de Brouwere (VITO)
and Frederik Verdonck (ARCHE)

Outline

- Introduction tiered approach
- Metal specific transfer factors
- Merlin-Expo: concepts and case study (As)
- Summary and possible way forward

Towards a tiered approach

Progress timeline



Refine for critical pathway only (sensitivity analysis!)

Tier 5: Full site-specific assessment

Tier 4: Include monitoring data

Tier 3: refined generic higher tier assessment

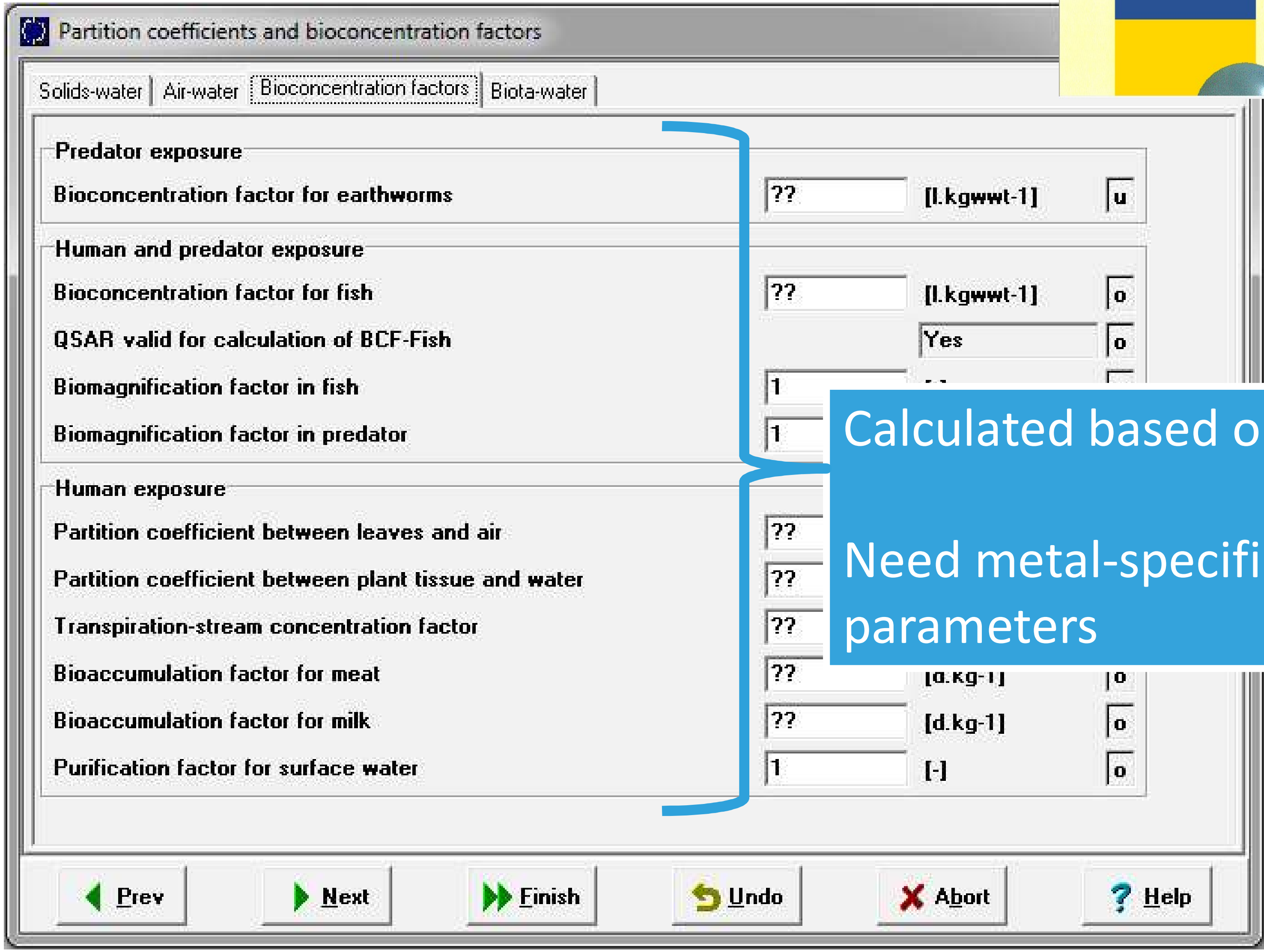
Tier 2: EUSES with metal-specific parameters

Tier 1: EUSES screening

Start

Tier 1

EUSES VERSION 2.1 European Union System for the Evaluation of Substances

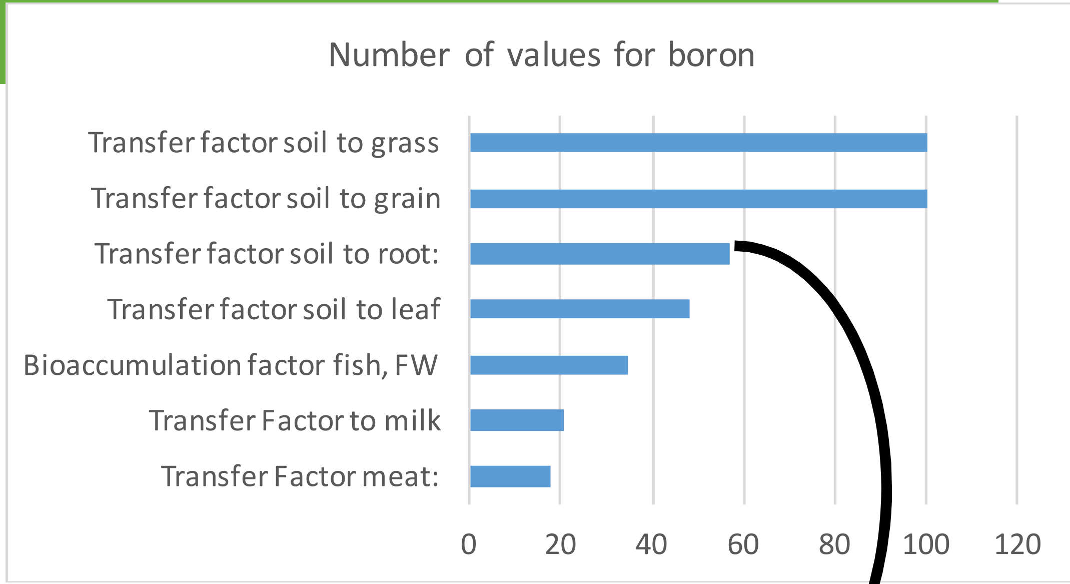


Calculated based on log Kow

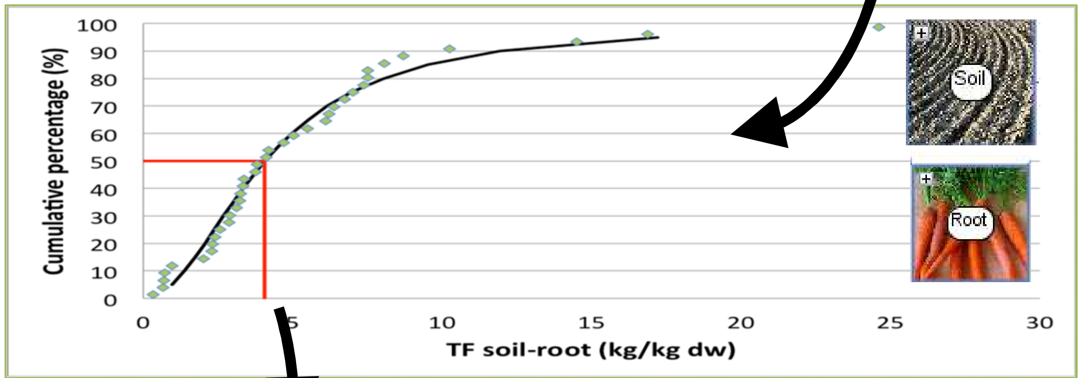
Need metal-specific parameters

Tier 2

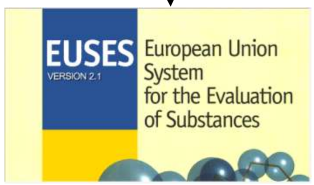
1. Collect data from literature



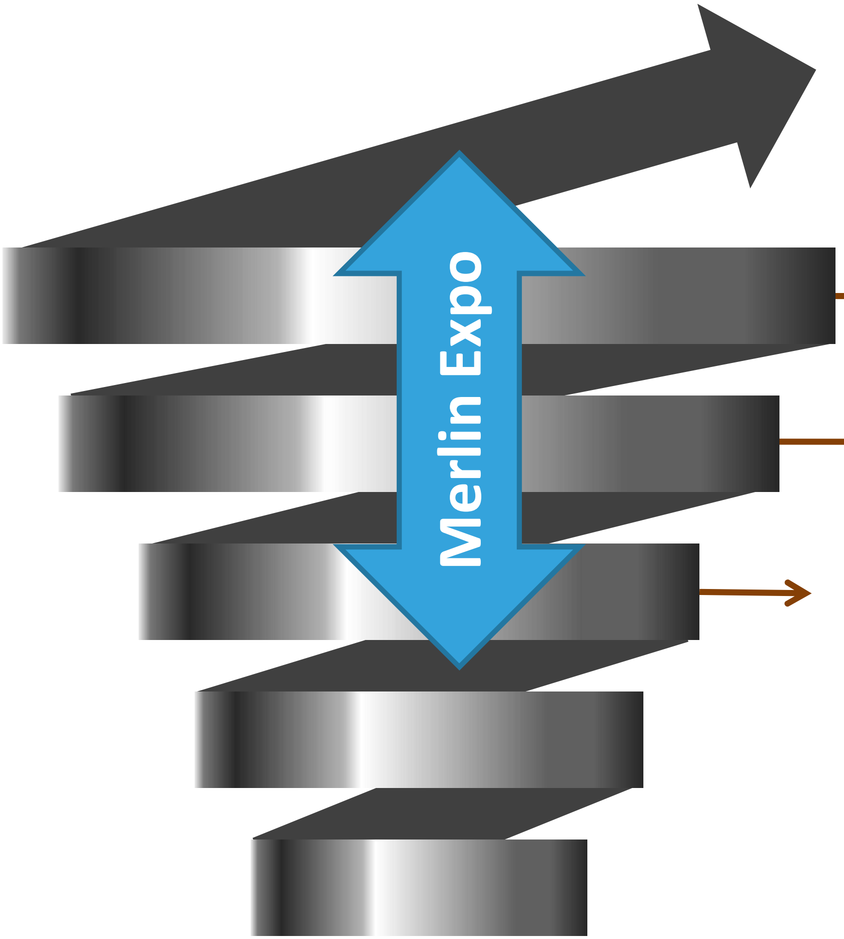
2. Consolidate (e.g. 50th percentile)



3. Input in EUSES



Use of Merlin Expo as a higher Tier tool ?



Tier 5: Full site-specific assessment

Tier 4: Include monitoring data

Tier 3: refined generic higher tier assessment

Start

MERLIN EXPO

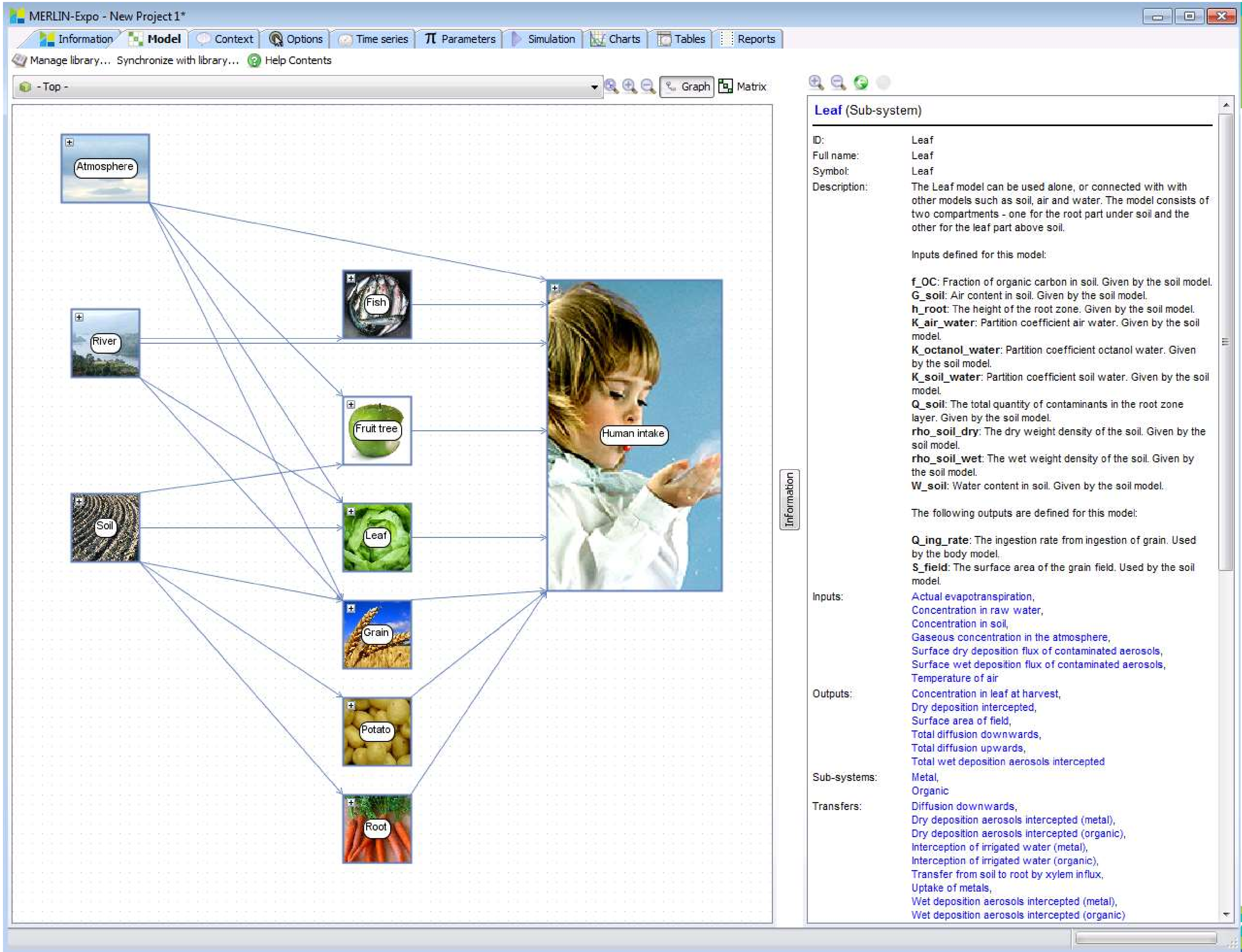
- **M**odelling **E**xposure to chemicals for **R**isk assessment: a comprehensive **L**ibrary of multimedia and PBPK models for **I**ntegration, Prediction, u**N**certainty and Sensitivity analysis.
- Freely available at http://merlin-expo.eu/
- Result from EU Research projects 2FUN & 4FUN

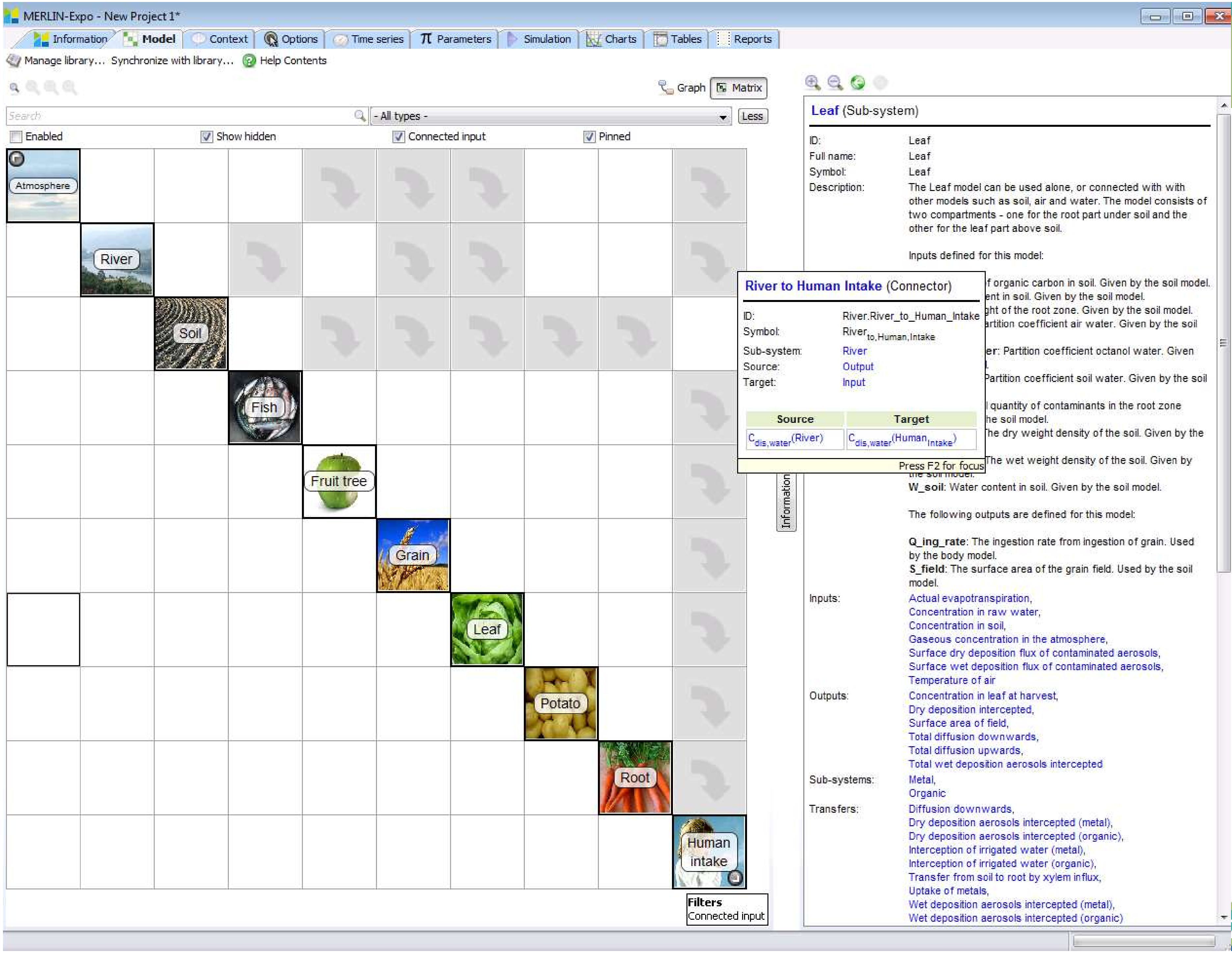
Consortium 4FUN project

What is MERLIN-Expo?

- Chemical Exposure Model, predicts:
  - Environmental and external human intake concentrations
  - Human internal (organs) concentrations
- Integrates:
  - Environmental multimedia model (river, soil, fruits, etc…)
  - PBPK model for fate in human body
- Uncertainty and sensitivity analysis
- Organics and metals

- Full documentation according to CEN standard
- Transparent model browsing
- e-learning platform


MERLIN-Expo - New Project 1*
Information
Model
Context
Options
Time series
Parameters
Simulation
Charts
Tables
Reports
Manage library…
Synchronize with library…
Help Contents
- Top -
Graph
Matrix
Atmosphere
River
Soil
Fish
Fruit tree
Leaf
Grain
Potato
Root
Human intake
Information
Leaf (Sub-system)
ID: Leaf
Full name: Leaf
Symbol: Leaf
Description: The Leaf model can be used alone, or connected with with other models such as soil, air and water. The model consists of two compartments - one for the root part under soil and the other for the leaf part above soil.
Inputs defined for this model:
f_OC: Fraction of organic carbon in soil. Given by the soil model.
G_soil: Air content in soil. Given by the soil model.
h_root: The height of the root zone. Given by the soil model.
K_air_water: Partition coefficient air water. Given by the soil model.
K_octanol_water: Partition coefficient octanol water. Given by the soil model.
K_soil_water: Partition coefficient soil water. Given by the soil model.
Q_soil: The total quantity of contaminants in the root zone layer. Given by the soil model.
rho_soil_dry: The dry weight density of the soil. Given by the soil model.
rho_soil_wet: The wet weight density of the soil. Given by the soil model.
W_soil: Water content in soil. Given by the soil model.
The following outputs are defined for this model:
Q_ing_rate: The ingestion rate from ingestion of grain. Used by the body model.
S_field: The surface area of the grain field. Used by the soil model.
Inputs: Actual evapotranspiration, Concentration in raw water, Concentration in soil, Gaseous concentration in the atmosphere, Surface dry deposition flux of contaminated aerosols, Surface wet deposition flux of contaminated aerosols, Temperature of air
Outputs: Concentration in leaf at harvest, Dry deposition intercepted, Surface area of field, Total diffusion downwards, Total diffusion upwards, Total wet deposition aerosols intercepted
Sub-systems: Metal, Organic
Transfers: Diffusion downwards, Dry deposition aerosols intercepted (metal), Dry deposition aerosols intercepted (organic), Interception of irrigated water (metal), Interception of irrigated water (organic), Transfer from soil to root by xylem influx, Uptake of metals, Wet deposition aerosols intercepted (metal), Wet deposition aerosols intercepted (organic)


MERLIN-Expo - New Project 1*
Information
Model
Context
Options
Time series
Parameters
Simulation
Charts
Tables
Reports
Manage library...
Synchronize with library...
Help Contents
Graph
Matrix
Search
- All types -
Less
Enabled
Show hidden
Connected input
Pinned
Atmosphere
River
Soil
Fish
Fruit tree
Grain
Leaf
Potato
Root
Human intake
Filters
Connected input
Information
River to Human Intake (Connector)
ID: River.River_to_Human_Intake
Symbol: River to,Human,Intake
Sub-system: River
Source: Output
Target: Input
Source
Target
Cdis,water(River)
Cdis,water(HumanIntake)
Press F2 for focus
Leaf (Sub-system)
ID: Leaf
Full name: Leaf
Symbol: Leaf
Description: The Leaf model can be used alone, or connected with with other models such as soil, air and water. The model consists of two compartments - one for the root part under soil and the other for the leaf part above soil.
Inputs defined for this model:
W_soil: Water content in soil. Given by the soil model.
The following outputs are defined for this model:
Q_ing_rate: The ingestion rate from ingestion of grain. Used by the body model.
S_field: The surface area of the grain field. Used by the soil model.
Inputs: Actual evapotranspiration, Concentration in raw water, Concentration in soil, Gaseous concentration in the atmosphere, Surface dry deposition flux of contaminated aerosols, Surface wet deposition flux of contaminated aerosols, Temperature of air
Outputs: Concentration in leaf at harvest, Dry deposition intercepted, Surface area of field, Total diffusion downwards, Total diffusion upwards, Total wet deposition aerosols intercepted
Sub-systems: Metal, Organic
Transfers: Diffusion downwards, Dry deposition aerosols intercepted (metal), Dry deposition aerosols intercepted (organic), Interception of irrigated water (metal), Interception of irrigated water (organic), Transfer from soil to root by xylem influx, Uptake of metals, Wet deposition aerosols intercepted (metal), Wet deposition aerosols intercepted (organic)

Tier 3

More complex model fate pathway equations

EUSES (Tier 2)

$C_{root} = TF_{soil\_root} \times C_{soil} \; / \; RHO_{soil}$

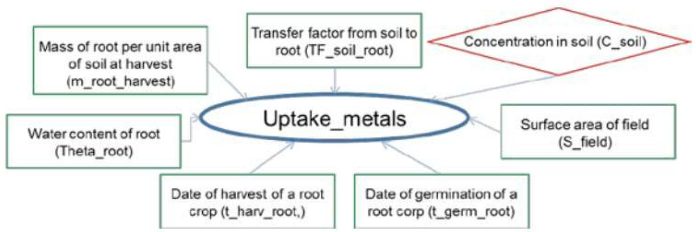
MERLIN-Expo (Tier 3)

The uptake of metals from soil into roots is governed by a substance-specific equilibrium transfer factor:

$$\frac{dC_{root}}{dt} = TF_{soil\_root} \times \frac{(1-\theta_{root})}{(t_{harv\_root} - t_{germ\_root})} \times m_{root\_harvest} \times C_{soil} \times S_{field}$$

Where

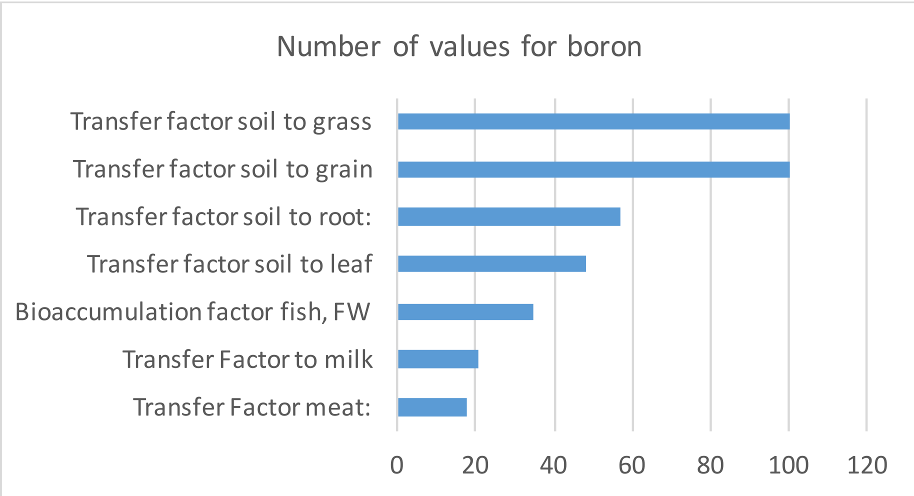
- ✓ $Uptake_{metals}$ ($mg\ d^{-1}$) : Uptake of metals
- ✓ TF_{soil_root} ($kg_{dw}\ kg_{dw}^{-1}$) : Transfer factor from soil to root
- ✓ Θ_{root} ($L\ kg_{fw}^{-1}$) : Water content of root
- ✓ t_{harv_root} (d) : Date of harvest of a root crop
- ✓ t_{germ_root} (d) : Date of germination of a root crop
- ✓ $m_{root\_harvest}$ ($kg_{fw}\ m^{-2}$) : Mass of root per unit area of soil at harvest
- ✓ C_{soil} ($mg\ kg_{dw}^{-1}$) : Concentration in soil (on dry mass basis)
- ✓ S_{field} (m^2) : Surface area of field



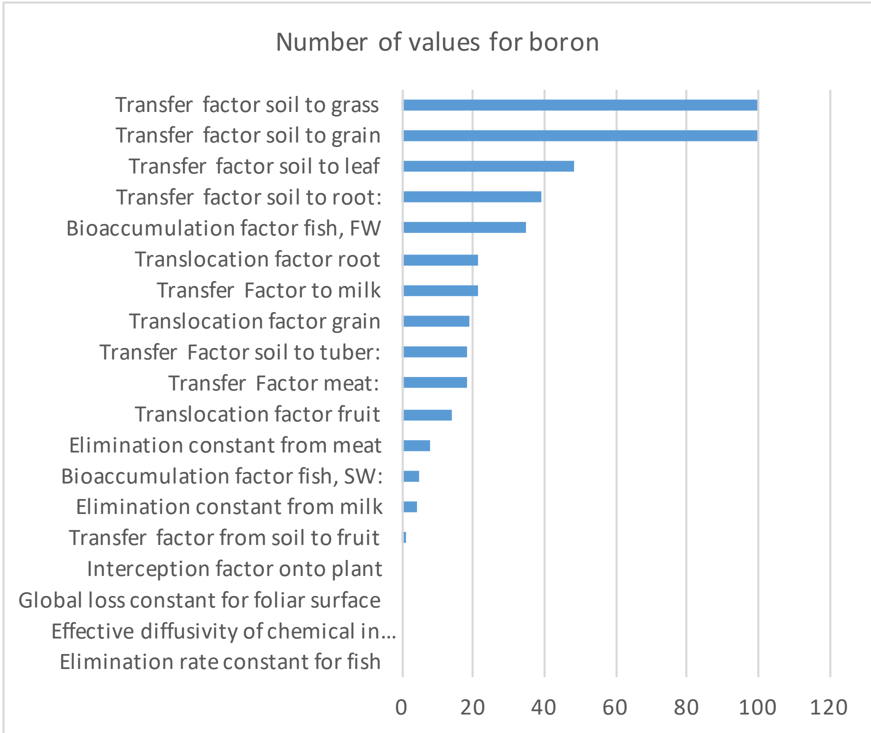
Tier 3

More fate parameters required

EUSES (Tier 2)



MERLIN-Expo (Tier 3)



Dietary intake assessment

More refined daily intakes can be added

EUSES (Tier 1 - 2)

HUMAN DAILY INTAKE OF FOOD AND WATER (FROM EUSES)	
Food	**Intake**
Drinking water	2 l/d
Fish	0.115 kg/d
Leaf crops (incl. fruit and cereals)	1.2 kg/d
Root crops	0.384 kg/d
Meat	0.301 kg/d
Dairy products	0.561 kg/d

MERLIN-Expo

Food and water intake: "empty box" in Merlin-Expo (no defaults for intake rates)

Possibility to implement from simple to complex food consumption patterns, such as:

- ESFA food consumption databases **(Tier 3 – 4)**
- Consumption data gathered in site specific surveys **(Tier 5)**

Dietary intake assessment

EFSA food consumption database: https://www.efsa.europa.eu/en/data/food-consumption-data

- based on 32 dietary surveys in 22 EU Member States
- infants, children, adolescent, adults and elderly
- common food classification system "FoodEx" (3 levels)

Country	Survey	Age_class	FoodExL2_code	HFoodExL2_code	FoodExL1_name	N_subjects	Mean	Std	P5	P10	Median
Belgium	Diet_National_2004	Adolescents	A.01.000001	A.01	Grains and grain-based products	584	258,8	129,8	79,8	114,1	240,3
Belgium	Diet_National_2004	Adolescents	A.01.000317	A.02	Vegetables and vegetable products (	584	94,1	85,4	0,0	3,0	76,0
Belgium	Diet_National_2004	Adolescents	A.01.000467	A.03	Starchy roots and tubers	584	91,9	84,3	0,0	0,0	70,5
Belgium	Diet_National_2004	Adolescents	A.01.000486	A.04	Legumes, nuts and oilseeds	584	7,2	18,1	0,0	0,0	0,0
Belgium	Diet_National_2004	Adolescents	A.01.000544	A.05	Fruit and fruit products	584	85,9	107,5	0,0	0,0	56,8
Belgium	Diet_National_2004	Adolescents	A.01.000727	A.06	Meat and meat products (including ed	584	110,3	81,1	12,4	24,0	94,5
Belgium	Diet_National_2004	Adolescents	A.01.000876	A.07	Fish and other seafood (including amp	584	14,8	29,4	0,0	0,0	0,0
Belgium	Diet_National_2004	Adolescents	A.01.000948	A.08	Milk and dairy products	584	212,7	202,6	0,0	13,0	157,0
Belgium	Diet_National_2004	Adolescents	A.01.001252	A.09	Eggs and egg products	584	9,5	20,2	0,0	0,0	0,0
Belgium	Diet_National_2004	Adolescents	A.01.001267	A.10	Sugar and confectionary	584	31,7	33,8	0,0	0,0	22,5
Belgium	Diet_National_2004	Adolescents	A.01.001346	A.11	Animal and vegetable fats and oils	584	18,9	20,5	0,7	2,2	12,3
Belgium	Diet_National_2004	Adolescents	A.01.001394	A.12	Fruit and vegetable juices	584	115,8	192,7	0,0	0,0	0,0
Belgium	Diet_National_2004	Adolescents	A.01.001470	A.13	Non-alcoholic beverages (excepting r	584	538,1	466,9	0,0	0,0	450,0
Belgium	Diet_National_2004	Adolescents	A.01.001534	A.14	Alcoholic beverages	584	65,4	259,3	0,0	0,0	0,0
Belgium	Diet_National_2004	Adolescents	A.01.001573	A.15	Drinking water (water without any addit	584	566,8	553,4	0,0	0,0	450,0
Belgium	Diet_National_2004	Adolescents	A.01.001580	A.16	Herbs, spices and condiments	584	44,6	54,9	0,0	0,0	28,1
Belgium	Diet_National_2004	Adolescents	A.01.001715	A.17	Food for infants and small children	584	0,4	3,2	0,0	0,0	0,0
Belgium	Diet_National_2004	Adolescents	A.01.001748	A.18	Products for special nutritional use	584	10,9	72,7	0,0	0,0	0,0
Belgium	Diet_National_2004	Adolescents	A.01.001789	A.19	Composite food (including frozen proc	584	78,4	115,1	0,0	0,0	20,0
Belgium	Diet_National_2004	Adolescents	A.01.001877	A.20	Snacks, desserts, and other foods	584	27,0	40,1	0,0	0,0	10,0
Belgium	Diet_National_2004	Adults	A.01.000001	A.01	Grains and grain-based products	1304	238,4	122,5	72,0	100,5	217,1
Belgium	Diet_National_2004	Adults	A.01.000317	A.02	Vegetables and vegetable products (	1304	122,8	99,6	0,0	11,4	105,0
Belgium	Diet_National_2004	Adults	A.01.000467	A.03	Starchy roots and tubers	1304	92,7	86,1	0,0	0,0	70,6
Belgium	Diet_National_2004	Adults	A.01.000486	A.04	Legumes, nuts and oilseeds	1304	10,3	23,7	0,0	0,0	0,0
Belgium	Diet_National_2004	Adults	A.01.000544	A.05	Fruit and fruit products	1304	117,8	119,5	0,0	0,0	90,5
Belgium	Diet_National_2004	Adults	A.01.000727	A.06	Meat and meat products (including ed	1304	120,8	84,7	15,7	28,9	105,5
Belgium	Diet_National_2004	Adults	A.01.000876	A.07	Fish and other seafood (including amp	1304	26,2	45,3	0,0	0,0	0,0
Belgium	Diet_National_2004	Adults	A.01.000948	A.08	Milk and dairy products	1304	172,3	167,8	0,0	19,5	132,5
Belgium	Diet_National_2004	Adults	A.01.001252	A.09	Eggs and egg products	1304	9,5	20,9	0,0	0,0	0,0
Belgium	Diet_National_2004	Adults	A.01.001267	A.10	Sugar and confectionary	1304	23,6	31,5	0,0	0,0	15,0
Belgium	Diet_National_2004	Adults	A.01.001346	A.11	Animal and vegetable fats and oils	1304	29,2	30,6	1,6	3,4	20,6
Belgium	Diet_National_2004	Adults	A.01.001394	A.12	Fruit and vegetable juices	1304	66,5	124,6	0,0	0,0	0,0
Belgium	Diet_National_2004	Adults	A.01.001470	A.13	Non-alcoholic beverages (excepting r	1304	742,2	552,1	125,0	215,7	625,0
Belgium	Diet_National_2004	Adults	A.01.001534	A.14	Alcoholic beverages	1304	216,6	391,9	0,0	0,0	62,5
Belgium	Diet_National_2004	Adults	A.01.001573	A.15	Drinking water (water without any addit	1304	675,6	624,8	0,0	0,0	565,0

Dietary intake assessment

Comparison of food consumption data : EUSES defaults vs. data in EFSA databases

Table 3.
Daily consumption data for Danish consumers of the age 4-5 years and 14-75 years (females), mean and 95th percentile for both groups, and consumption data suggested in the TGD.

Food type	4–5		14–75 (♀)		TGD
	Mean	95th	Mean	95th	
Root vegetables (g/d)	30	54	43	89	384[c]
Potatoes (g/d)	56	137	90	198	
Lettuce (g/d)	6	11	9	18	1200[d]
Other leafy veg. (g/d)	7	13	10	21	
Tree fruits (g/d)	111	235	137	318	
Cereal products (g/d)	185	269	195	309	
Milk (g/d)	448	796	303	754	561
Meat (non-poultry) (g/d)	76	138	89	166	301

Connect with MerlinExpo module ‘potato’, ‘grain’, ‘fruit tree’

Source : Legind et al. (2009) Environmental Pollution (Vol 157 778 – 785)
“modelling the exposure of children and adults via diet to chemicals in the environment with crop-specific models”

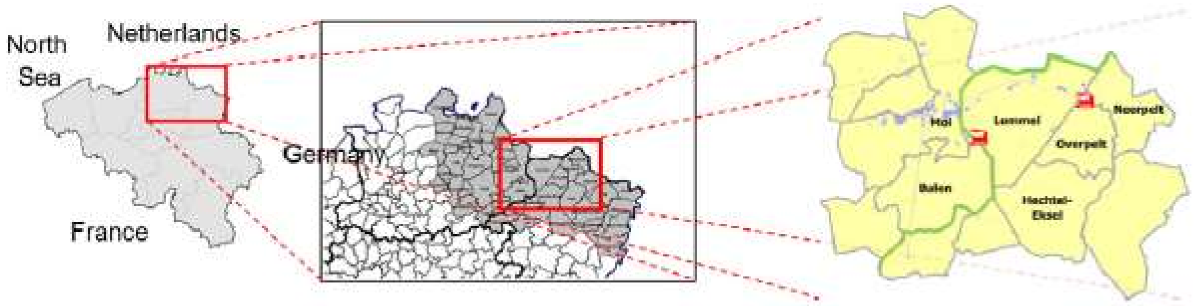
Use of monitoring data (Tier 4)

- Bypass modelling transfer environment → food
- Some examples where monitoring in food have been used in MvE exposure assessment REACH CSR:
  - Regional exposure assessment Nickel
  - Local exposure assessment Nickel
    - monitoring levels of Ni in lettuce and wheat grown around a Ni smelter
    - worst case: rather old data – high deposition levels
  - Local exposure assessment *Metal*
    - monitoring levels of *Me* in locally grown vegetables/fruit and drinking water from mining area
    - worst-case: overestimation of *Metal* industrial uses
- MerlinExpo: flexibility to use either modelled or monitoring data in food

Use of MerlinExpo at Tier 5

- Full site specific assessment using MerlinExpo:

  - Case study : “ assessing MvE exposure to inorganic As in Northern Campine area”
  - Context: past emissions by non-ferrous smelters (outside REACH)

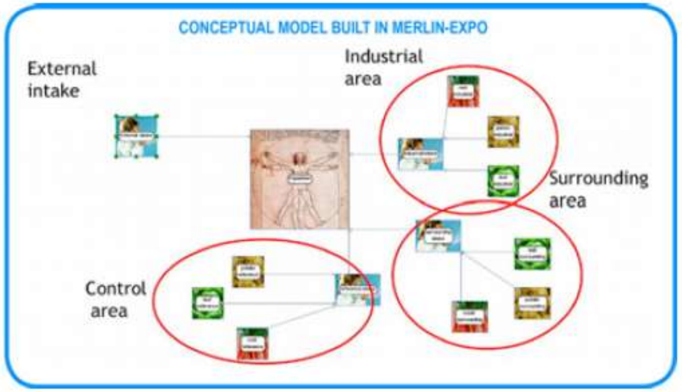


- Wealth of data on metal levels in environment and humans in this area
- Aim: demonstration MerlinExpo as a high tier exposure tool for site specific MvE exposure assessment

Use of MerlinExpo at Tier 5

STEP 1: Model set up in MerlinExpo

- Select building blocks and draw connections for study area

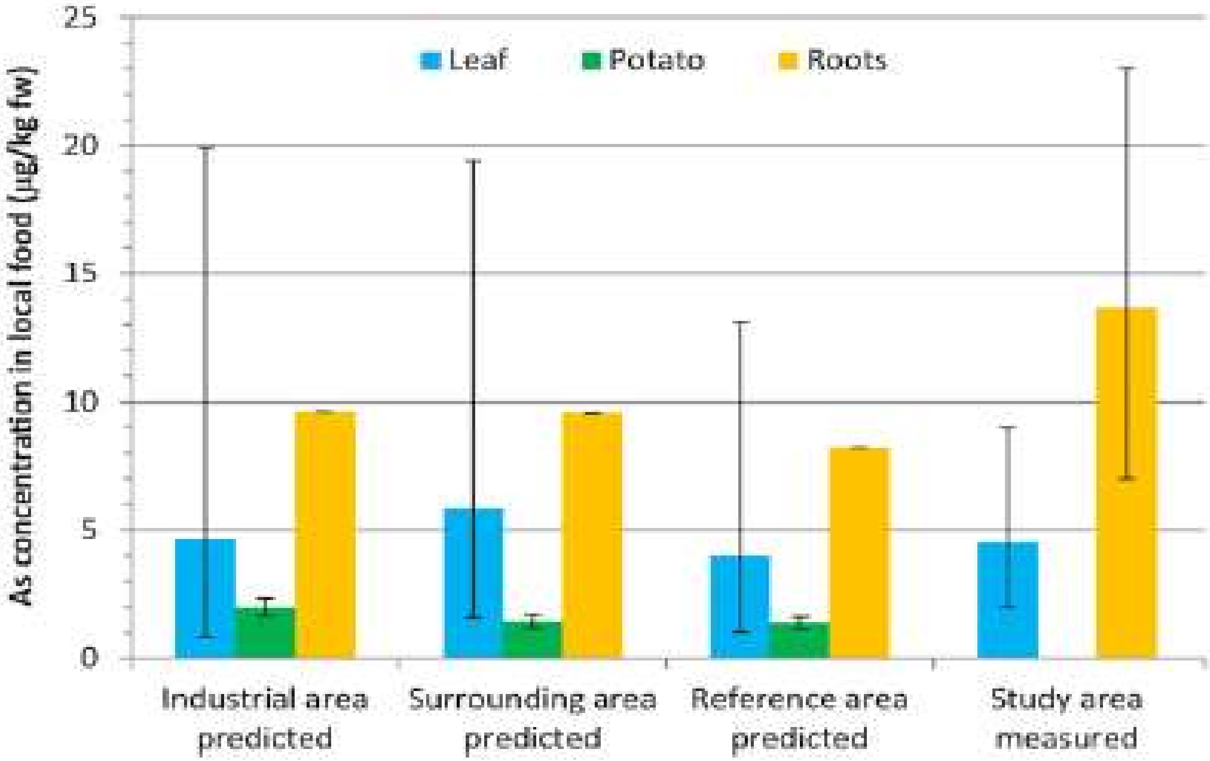


STEP 2: Model input and parameterization

- Site specific input data:
  - Environmental monitoring data : As levels in soil, dust, air, deposition, locally grown foods, imported food (source: from monitoring campains run in the study area)
  - Human related data: food consumption patterns, time-activity patterns, current and past home location (source: questionnaires completed by the participants recruited in the study area)
- generic model parameters:
  - e.g. for PBPK model (As), crop models (e.g. evapotranspiration, As soil – crop transfer factors); dust and soil ingestion rates, concentrations in non locally grown crops (source: literature)

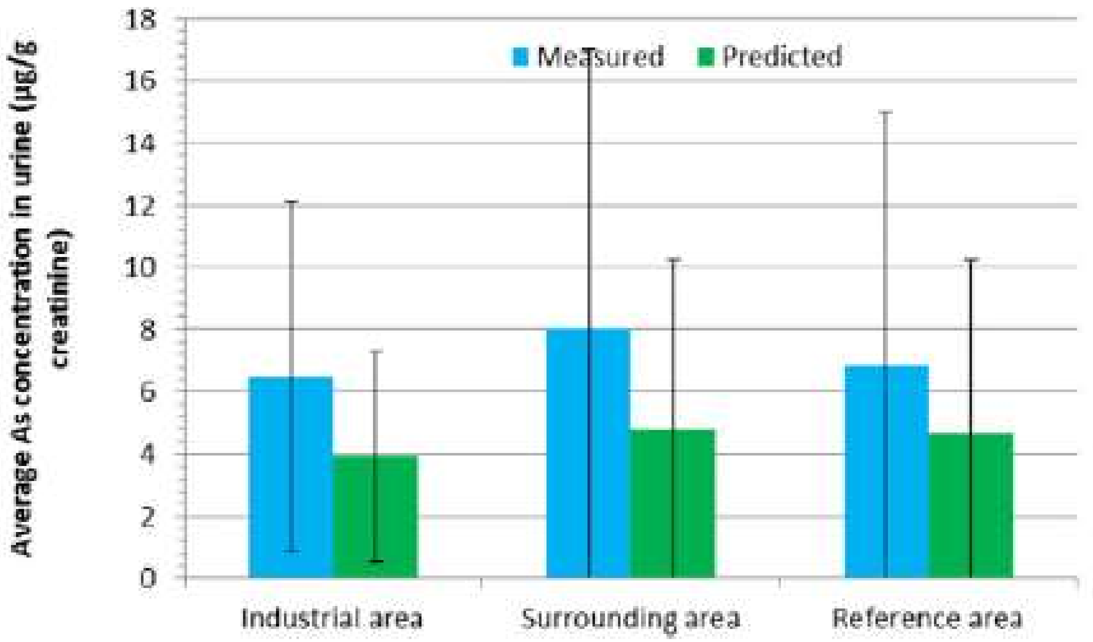
Use of MerlinExpo at Tier 5

STEP 3: model runs and comparison with monitoring data



Use of MerlinExpo at Tier 5

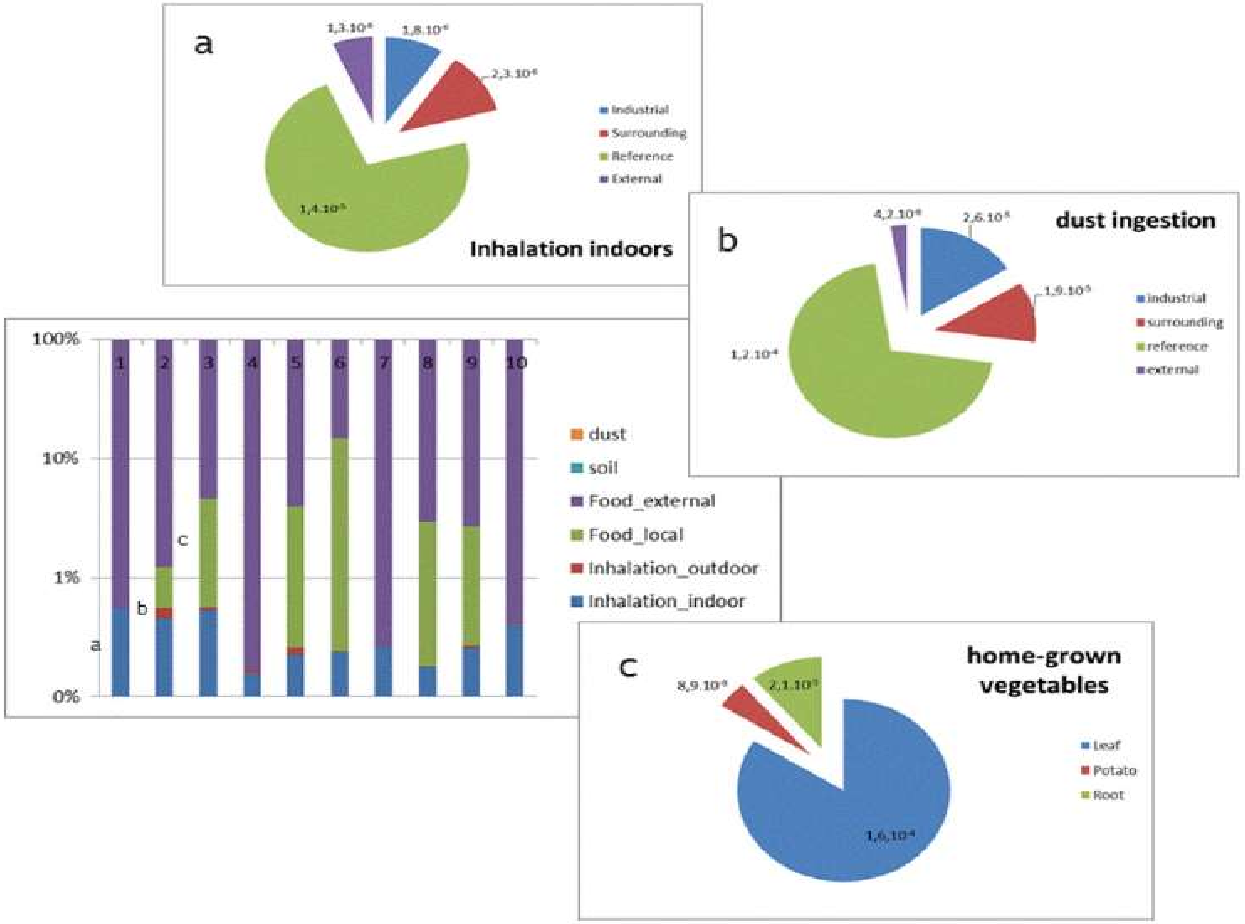
STEP 3: model runs and comparison with monitoring data



Source: Sci Tot Env Vol 568: 794 -802 (Van holderbeke et al., 2016)

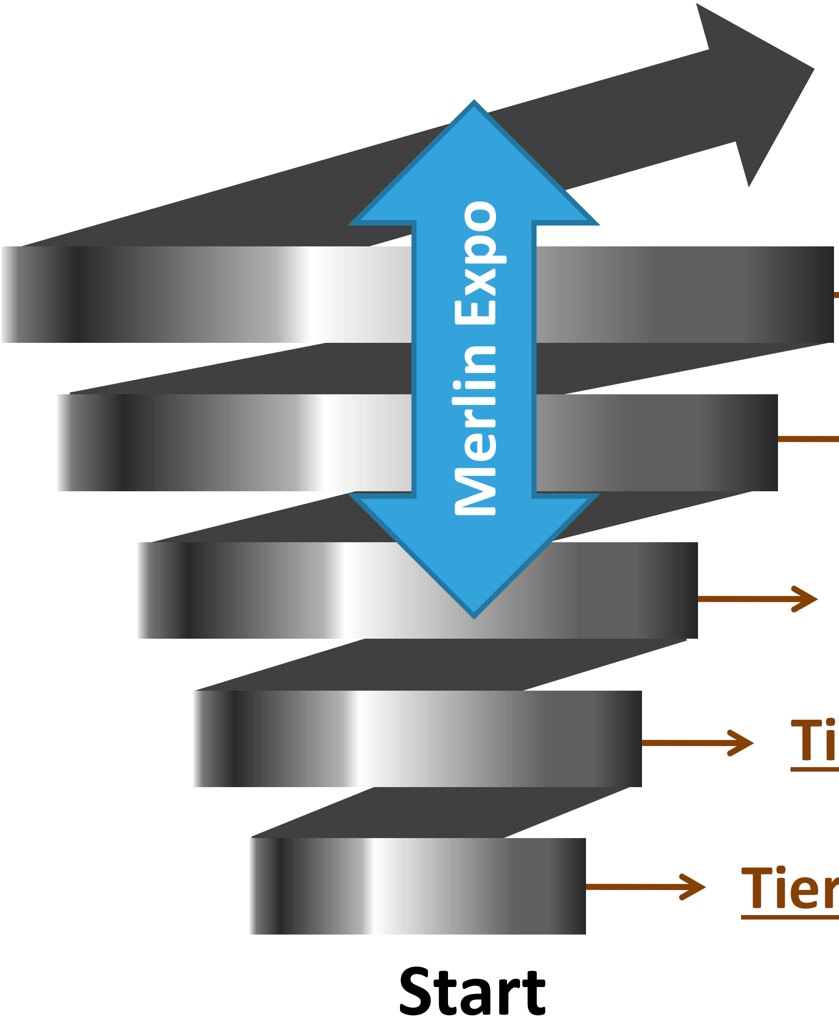
Use of MerlinExpo at Tier 5

Merlin expo modelling results: analyse of contribution of different exposure pathways and sources



Summary

Progress timeline



Refine for critical pathway only (sensitivity analysis!)

Tier 5: Full site-specific assessment

Tier 4: Include monitoring data

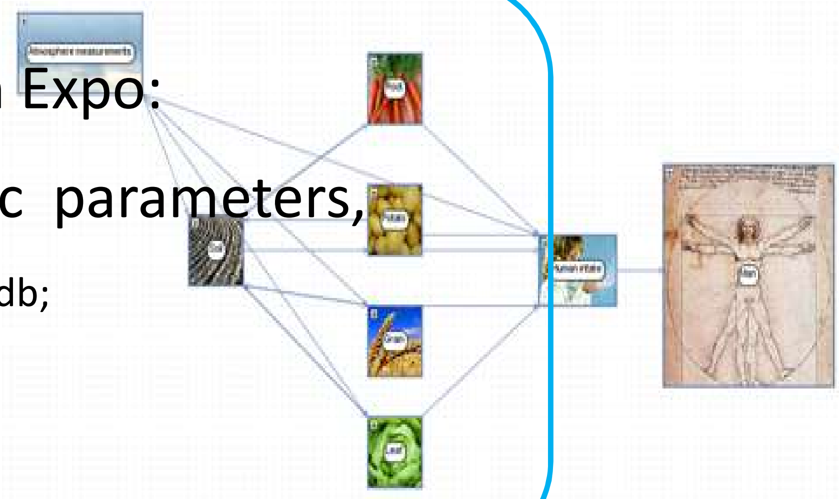
Tier 3: refined generic higher tier assessment

Tier 2: EUSES with metal-specific param.

Tier 1: EUSES screening

Use of Merlin Expo as Tier 3 tool for REACH ?

1. Setting up default scenario in Merlin Expo:
2. Fed the default scenario with generic parameters,
   - Typical EU dietary pattern based on EFSA db;
   - crop parameters
   - exposure factors
   - climatological factors,...



3. Set of metal/substance specific defaults
4. Set of case-specific required input parameters, aligned as much as posssible with data from CSR, e.g. PECsoil, PECair, etc.

4. Discussion and Way Forward

1. **What are the main data gaps** to improve scientifically, for metals and inorganics
2. **What are the most relevant tiered data levels** to improve the MvE assessment for metals
3. **What tiered modeling features could be improved and is MERLIN-expo a good tool** for assessing MvE for metals

Conclusions and closure

By co-chairs